=> d his

```
(FILE 'HOME' ENTERED AT 14:42:44 ON 09 SEP 2000)
    FILE 'HCAPLUS' ENTERED AT 14:43:07 ON 09 SEP 2000
           222 S SHAN J?/AU
1.1
L2
          6308 S WU X?/AU
L3
           400 S LING L?/AU
           389 S PANG P?/AU
L4
L5
             1 S L1 AND L2 AND L3 AND L4
               SELECT RN L5 1
                                                                      search
    FILE 'REGISTRY' ENTERED AT 14:44:19 ON 09 SEP 2000
           12 S E1-12 12 cpd5 in L5 cite
L6
    FILE 'HCAPLUS' ENTERED AT 14:44:33 ON 09 SEP 2000
            1 s L5 AND L6 1 cite w/ 12 cpds dizyla yea
L7
L8
          7284 S L1-4
L9
            1 S L8 AND HYPERIC?
             0 S L9 NOT L7
    FILE 'REGISTRY' ENTERED AT 14:47:00 ON 09 SEP 2000
L11
              STR 55954-61-5 parent
L12
            12 S L11
           183 S L11 FUL 183 Cpd5
L13
              SAVE L13 MEL572P/A
    FILE 'REGISTRY' ENTERED AT 14:50:03 ON 09 SEP 2000
    FILE 'HCAPLUS' ENTERED AT 14:53:35 ON 09 SEP 2000
           513 S L13 513 cites
136 S L14(L)THU/RL
                                      for 413 136 cites autinhed to a
L15
                                                                            the opute rolp
           214 S T-TYPE CALCIUM CHANNEL
L16
        292644 S DEPRESSION OR HEART FAILURE OR CHF OR ISCHAEM? OR ISCHEM? OR
L17
L18
            1 S L15 AND L16
L19
            12 S L15 AND L17
L20
           12 S L19 OR L18
                            11 cites related to a dained use
           11 S L20 NOT L7
    FILE 'REGISTRY' ENTERED AT 15:04:14 ON 09 SEP 2000
    FILE 'STNGUIDE' ENTERED AT 15:08:20 ON 09 SEP 2000
    FILE 'REGISTRY' ENTERED AT 15:14:15 ON 09 SEP 2000
L22
              STR 147593-87-1
L23
           11 S L22 SSS SAM SUB=L13
                                    148 cpds posed on U2
           148 S L22 SSS FUL SUB=L13
              SAVE L24 MEL572S1/A
    FILE 'HCAPLUS' ENTERED AT 15:38:09 ON 09 SEP 2000
         510 S L24
                       510 cites
L25
    FILE 'REGISTRY' ENTERED AT 15:39:01 ON 09 SEP 2000
    FILE 'STNGUIDE' ENTERED AT 15:39:56 ON 09 SEP 2000
    FILE 'REGISTRY' ENTERED AT 15:51:44 ON 09 SEP 2000 STR 55954-61-5
L26
              STR L26
L27
L28
              STR L26
1.29
              STR L28
           2 S L26-29 SSS SAM SUB=L24
36 S L26-29 SSS FUL SUB=L24 36 epds based on A-D provisols of Cl 18
L30
            2 S L26-29 SSS SAM SUB=L24
    FILE 'HCAPLUS' ENTERED AT 16:04:49 ON 09 SEP 2000
L32
           476 S L31
    FILE 'REGISTRY' ENTERED AT 16:05:19 ON 09 SEP 2000
```

SEARCHED BY SUSAN HANLEY 305-4053

Page 1

112 cpds afta compounds subtacting stars of LZ MELLER 09/481,572 1.12. SHID24ENOTES1 = A-D Provisors of UIS FILE 'HCAPLUS' ENTERED AT 16:05:59 ON 09 SEP 2000

93 S L33

10 S L33 Lates for remains cpd S

10 S L33 Lates for remains cpd S

SELECT RN L35 1-10

10 cites related to a theraputic ro/e L34 65 S E13-77
75 S L6 OR L36) these are all the cpds displayed 80 far;
93 S L33 NOT L37 = there gpds are subtracted to avoid L37 L38 FILE 'HCAPLUS' ENTERED AT 16:13:46 ON 09 SEP 2000

68 \$ L38 68 cites for L38

FILE 'REGISTRY' ENTERED AT 16:16:11 ON 09 SEP 2000

STR L29

STR L40

1 \$ L40 OR L41 SSS FUL SUB=L24 I cpd for Port from Original L2

93 \$ L38 NOT L42 \$ fill 93 cpds after subtract Set

128 \$ L44 SSS SAM SUB=L24

128 \$ L44 SSS FUL SUB=L24 Cpds for C120

Ont 1 L39 L40 L41 1.42 L45 128 S L44 SSS FUL SUB=L24 Cpds for CL26 FILE 'HCAPLUS' ENTERED AT 16:33:32 ON 09 SEP 2000 FILE 'REGISTRY' ENTERED AT 16:40:37 ON 09 SEP 2000 L47 105 S L46 NOT L37 FILE 'HCAPLUS' ENTERED AT 16:40:57 ON 09 SEP 2000 FILE 'REGISTRY' ENTERED AT 16:42:47 ON 09 SEP 2000 77 S L47 NOT L31 = 77 cpds for Cl 20 after subtracting out

(HCAPLUS' ENTERED AT 16:43:11 ON 09 SEP 2000

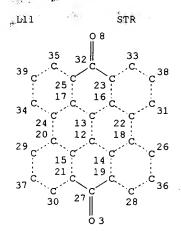
63 S L48 63 cites

1 S L49 AND PY>1999

62 S L49 NOT L50 62 cites of Pubyear C2000

03 S L49 NOT L50 62 cites of Pubyear C2000 FILE 'HCAPLUS' ENTERED AT 16:43:11 ON 09 SEP 2000
63 S L48 63 c 1+6 5
1 S L49 AND PY>1999 L49 L50 L51 0 S L51 AND (L16 OR L17)
1 S L51 (L) THU/RL | Cite linked to theapy L52 s L51 (L) THU/RL | Cites ; 1-31 displayed; the remaining save L54 MEL572HC/L Cites; 1-31 displayed; the remaining cites are saved if you want them £53 61 S L51 NOT L53

=> d que 114



parent STR

all gites open to

substract 3,8

this is TR was used for the

method claim in order to preh

up possible 103's

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

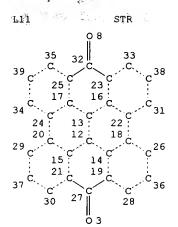
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

L13 183 SEA FILE=REGISTRY SSS FUL L11

L14 513 SEA FILE=HCAPLUS ABB=ON PLU=ON L13

=> d que 125



parent STR

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

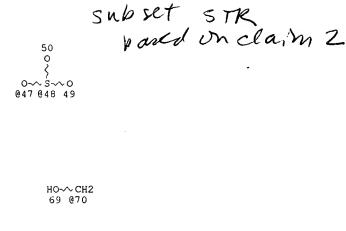
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

L13 183 SEA FILE=REGISTRY SSS FUL L11 L22 STR

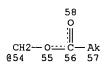
043 44 45 40 : 35 32 18 35 6 G3 25 21 19 27 15 16 30 37 20 22 38 .Ċ_{\\}G2 42 11 G2

Ö 2



CH2—O—Ak @51 52 53

G1 3



Ġ1 5

O√Ak @59 60



Page 1-A

Page 2-A

VAR G1=H/OH/59/43 VAR G2=H/AK/X/47/48 VAR G3=H/AK/OH/59/43/70/51/54/62/66 NODE ATTRIBUTES: CONNECT IS E1 RC AT 68 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE

L24 148 SEA FILE=REGISTRY SUB=L13 SSS FUL L22 L25 510 SEA FILE=HCAPLUS ABB=ON PLU=ON L24

≢> d'que 132 STR pare 33 .с³⁸ 22 : 18 21 19 30 28

this part of the search is to subtract out the provisos of cl. 18

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

öз

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 30

28

Ö2

G1 3

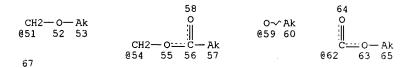
31

G1 5

STEREO ATTRIBUTES: NONE

183 SEA FILE=REGISTRY SSS FUL L11 L13 L22 STR

Subset 5TR For claim 2 46 0 12 G2 – Ak 0~ s~0 G2 41 043 44 45 @47 @48 49 26 40 32 18 35 6 G3 G3 9 25 21 G3 4 27 15 16 30 HO-√ CH2 20 22 38 69 070



G2 42

Page 1-A

11 G2

Page 2-A

VAR G1=H/OH/59/43
VAR G2=H/AK/X/47/48
VAR G3=H/AK/OH/59/43/70/51/54/62/66
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 68
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE

148 SEA FILE=REGISTRY SUB=L13 SSS FUL L22

L24 148 SEA L26 STR

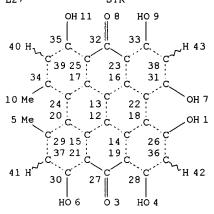
08 HO 9 OH 11 39 25 C 23 38 16 34 17 31 10 HO 13 22 12 18 5 HO, Me 1 29 15 C 26 14 37 21 C 19 36 H 42 30 27 28 öз HÒ 6 HO 4

These are the proviso subset 5TR's

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE L27 STR

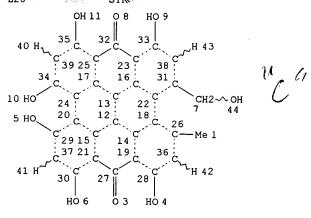


"B

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 42 STEREO ATTRIBUTES: NONE L28 STR

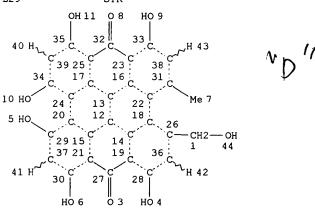
more proviso substrats
for £ cl 18



NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE L29 STR



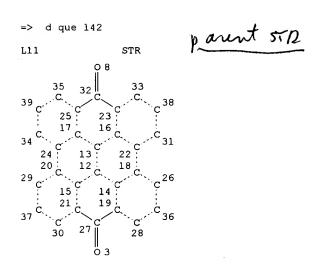
NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE

L31 36 SEA FILE=REGISTRY SUB=L24 SSS FUL (L26 OR L27 OR L28 OR L29)

L32 476 SEA FILE=HCAPLUS ABB=ON PLU=ON L31



I for got to subsect of for out the subsect of for the "E' i "F" provisors of Cl 18

STOR Vared on Cla

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE 183 SEA FILE=REGISTRY SSS FUL L11 subset L13 L22 STR 50 G1 10 07 0 G2 41 @47 @48 49 40 18 35 6 G3 G3 9 25 23 21 G3 4 27 15 16 30 HO-√ CH2 22 37 20 38 69 070 ¹G2 42 11 G2 28 31 Ö 2 G1 3 G1 5 58 64 0 0 CH2-0-Ak O-√Ak 52 53 @59 60 -- O--- Ak CH2-- o---- "C-55 56 57 63 65 054 062 67

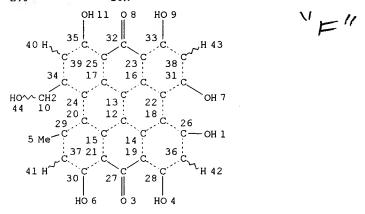
Page 2-A

VAR G1=H/OH/59/43 VAR G2=H/AK/X/47/48 VAR G3=H/AK/OH/59/43/70/51/54/62/66 NODE ATTRIBUTES: CONNECT IS E1 RC AT 68 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE

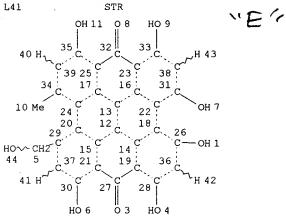
L24 148 SEA FILE=REGISTRY SUB=L13 SSS FUL L22 L40 STR



NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE



NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE L42 1 SEA FILE=REGISTRY SUB=L24 SSS FUL L40 OR L41

only 1 apd

This display shows the opds for cl 20 after Subtracting out previously displayed apds

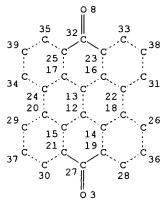
=> d que 148

L6

12 SEA FILE=REGISTRY ABB=ON PLU=ON (548-04-9/BI OR 11079-53-1/BI OR 117-39-5/BI OR 143183-63-5/BI OR 153-18-4/BI OR 1617-53-4/B I OR 21637-25-2/BI OR 482-36-0/BI OR 52-39-1/BI OR 522-12-3/BI OR 55954-61-5/BI OR 9004-10-8/BI)

opds from in ventor seure

L11



STR

parent STR

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

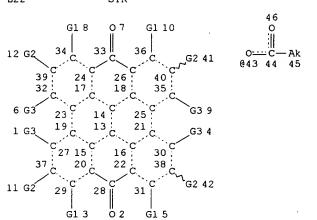
GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 30

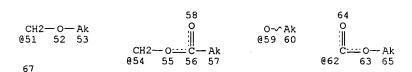
STEREO ATTRIBUTES: NONE

L13 183 SEA FILE=REGISTRY SSS FUL L11 L22 STR

HO-√ CH2

69 @70





Page 1-A

0 || || || || || || || ||

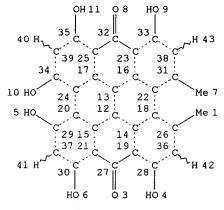
Page 2-A
VAR G1=H/OH/59/43
VAR G2=H/AK/X/47/48
VAR G3=H/AK/OH/59/43/70/51/54/62/66
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 68
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 69

STEREO ATTRIBUTES: NONE

L24 L26 148 SEA FILE=REGISTRY SUB=L13 SSS FUL L22

6 STR

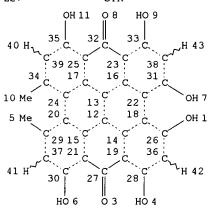


proviso and MA11 of Cl 18

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE L27 STR



proviso "B" of UF18

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE L28 STR OH 11 0.8 но 9 33 38 C 23 39 25 34 17 16 31 10 HO CH2∼ OH 44 20 12 18 5 HO 29 15 14 37 21 C 19 41 H 30 27 28

öз

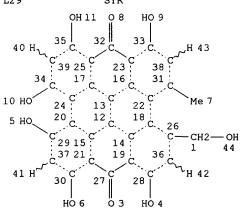
provisso "e" of el 18

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

но 6

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE L29 STR



proviso "D" of Ce 118

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE

L31 36 SEA FILE=REGISTRY SUB=L24 SSS FUL (L26 OR L27 OR L28 OR L29)
L36 65 SEA FILE=REGISTRY ABB=ON PLU=ON (548-04-9/BI OR 120667-79-0/B

SEARCHED BY SUSAN HANLEY 305-4053

I OR 147593-87-1/BI OR 147593-89-3/BI OR 121263-19-2/BI OR 137363-72-5/BI OR 141436-78-4/BI OR 157301-83-2/BI OR 35082-49 6/BI OR 55954-61-5/BI OR 60483-14-9/BI OR 109-86-4/BI OR 111-77-3/BI OR 127180-29-4/BI OR 130942-84-6/BI OR 137632-06-5/ BI OR 138674-26-7/BI OR 140208-17-9/BI OR 144700-81-2/BI OR 144788-48-7/BI OR 144941-32-2/BI OR 145987-20-8/BI OR 151765-07 -0/BI OR 151765-17-2/BI OR 151766-28-8/BI OR 155092-33-4/BI OR 160919-80-2/BI OR 160919-81-3/BI OR 160919-82-4/BI OR 160919-83 -5/BI OR 160919-84-6/BI OR 160919-85-7/BI OR 160919-86-8/BI OR 160919-87-9/BI OR 160919-88-0/BI OR 160919-89-1/BI OR 164397-05 -1/BI OR 164397-06-2/BI OR 168323-98-6/BI OR 168323-99-7/BI OR 171782-05-1/BI OR 18521-72-7/BI OR 185672-52-0/BI OR 189113-18-6/BI OR 189113-21-1/BI OR 189113-23-3/BI OR 189113-25-5/BI OR 189113-27-7/BI OR 19267-89-1/BI OR 19697-87-1/BI OR 20516-32-9/ BI OR 20752-80-1/BI OR 475-64-9/BI OR 481-70-9/BI OR 481-74-3/B I OR 518-82-1/BI OR 521-61-9/BI OR 52660-18-1/BI OR 55914-74-4/ BI OR 602-06-2/BI OR 60935-17-3/BI OR 66-97-7/BI OR 79079-06-4/ BI OR 88201-45-0/BI OR 9026-43-1/BI)

46

0

0---C-Ak @43 44 45 epds allready
bisplayed

L37 75 SEA FILE=REGISTRY ABB=ON PLU=ON L6 OR L36
L44 STR

G1 10 G1 8 07 33 36 12 G2 G2 41 40 39 24 26 18 35 32 17 `G3 9 6 G3 25 21 19 27 15 30 16 38 37 20 22 11 G2 28 0 2 G1 3 G1 5

CH2-O-Ak @51 52 53 opds of ce 20

Ak @71

58 O O Ak HO CH2 # 659 60 69 670 CH2-O---C-Ak 654 55 56 57

VAR G1=H/OH/59/43 VAR G2=H/71 VAR G3=H/71/OH/43/59/70/51/54 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM IS LOC ΑT 45 **GGCAT** 53 IS LOC GGCAT IS LOC ΑT 57 **GGCAT** 60 GGCAT IS LOC AΤ IS LOC ΑT 71 **GGCAT** DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 59

STEREO ATTRIBUTES: NONE

77 cpds for CL 20

 $G_1 = R_1 = R_2 = R_6 = R_{12} + \frac{1}{0}H/0R/0-E G_2 R_2 = R_5 = R_8 = R_{11} + \frac{1}{A}K/X/sogH$ $G_3 R_3 = R_4 = R_9 = R_{10} = \frac{1}{0}$ H/AK/0H/0R/0-ER/0-ER/cH20H/cH20R $CH_2O-E-R - E-0H/R$

```
ANSWER 16 OF 16 WPIDS COPYRIGHT 2000
                                             DERWENT INFORMATION LTD
L6
     1966-18731F [00]
                       WPIDS
AN
     Rheumatism treatment.
TI
DC
     B00
PA
     (TONE) TONERO A
CYC
                               (196800)*
ΡI
     BE 654914
                  Α
           654914 A UPAB: 19930831
AΒ
     Compns. containing as active agents extracts from ST. John's Wort
     (I) (Hypericum perforatum) and meadowsweet (II)
     ulmaria) in ratios 20-60% and 40-80% respectively in the form of
     balms and ointments.
           Treatment of rheumatism, angina, cardiac conditions,
     phlebitis, blood circulation conditions, psoriasis etc.
           Compns. contng. 20-60\% (I) and 40-80\% (II) as under
     "Composition".
     CPI
FS
FA
     AΒ
```

CPI: B04-A07F; B12-A07; B12-D07; B12-D09; B12-E01; B12-F01; B12-F02

MC

The Structure

L54 ANSWER 1 OF 61 HCAPLUS COPYRIGHT 2000 ACS

ΑN 1999:762921 HCAPLUS

DN 132:78375

TΙ From the photosensitizer hypericin to the photoreceptor stentorin-the chemistry of phenanthroperylene quinones

Falk, Heinz

Institut fur Chemie der Johannes Kepler Universitat, Linz, A-4040, Austria Angew. Chem., Int. Ed. (1999), 38(21), 3117-3136 CS SO CODEN: ACIEF5; ISSN: 1433-7851

Wiley-VCH Verlag GmbH PB

DT Journal; General Review

English LA

A review with 64 refs. on the chem. of phenanthroperylene quinones from the photosensitizer hyperican to the photoreceptor stentorin. The pursuit of the chem. of \natural compds. contg. phenanthroperylene quinones substituted with hydroxyl and alkyl groups dates back nearly half a century. It experienced a renaissance within the last decade when it turned out that one of these compds., hypericin isolated from St. Johns wort-a phytotherapeutic drug known since antiquity-does not only exhibit ingestion deterrence, but also antiviral, photodynamically useful, and sedative properties. The fact that this group of phenanthroperylene quinones also contains the photosensory pigments of protozoa, such as stentorin, has addnl. contributed to this new interest in this class of compds. However, It is also the wealth of chem. and phys. problems that spurred the curio rity of scientists to probe the phenanthroperylene quinones in more detail. These problems are mainly a result of the network of tautomerism, dissocn., conformation, and assocn. equil. and the structural complexity thus caused by them. In keeping with the broad array of interdisciplinary investigations, which reach from synthetic org. chem. and spectroscopy to physiol. and medicine, this review will focus on a picture of the chem. aspects of this fascinating class of mols. framed by the background of its biol. aspects.

147395-58-2, Stentorin RL: BOC (Biological occurrence); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PROC (Process)

(chem. aspects of phenanthroperylene quinones from the photosensitizer hypericin to the photoreceptor stentorin)

RN 147395-58-2 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

RE.CNT 278

- (1) Agostinis, P; Biochem Biophys Res Commun 1996, V220, P613 HCAPLUS
- (2) Agostinis, P; Biochem Pharmacol 1995, V49, P1615 HCAPLUS
- (3) Ahrer, W; Monatsh Chem 1998, V129, P643 HCAPLUS
- (4) Ali Al-Akhras, M; J Photochem Photobiol B 1996, V34, P169 HCAPLUS
- (5) Altmann, R; Monatsh Chem 1997, V128, P361 HCAPLUS ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr 154 2

ANSWER 2 OF 61 HCAPLUS COPYRIGHT 2000 ACS L54

1999:134526 HCAPLUS AN

DN 130:296542

ΤI Concerning regioselective photochemical intermolecular proton transfer from hypericin

AU Obermueller, Roland A.; Schuetz, Gerhard J.; Gruber, Hermann J.; Falk,

Inst. Chem., Johannes Kepler Univ., Linz, A-4040, Austria Monatsh. Chem. (1999), 130(2), 275-281 CODEN: MOCMB7; (SSN:)0026-9247 CS

SO

PB Springer-Verlag Wien

DT Journal

LA English

Using epifluorescence microscopy on lipid vesicles contg. hypericin or AB several of its O-alkylated derivs. together with a fluorescence pH indicator, it was shown that upon excitation of the resp. hypericinate ion an excited-state-derived proton is transferred to the indicator mol. In addn., it could also be unequivocally derived that this proton originates from one of the peri-hydroxyl groups of the pigment. 223115-06-8 223115-11-5

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process)

(regioselective photochem. intermol. proton transfer from hypericin)

223115-06-8 HCAPLUS RN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis(benzoyloxy)-1,6,8,13-tetrahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RN 223115-11-5 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis(benzoyloxy)-1,6,8,13-tetramethoxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RE.CNT 31

RE

- (1) Agostinis, P; Biochem Biophys Res Commun 1996, V220, F613 HCAPLUS
- (2) Altmann, R; Monatsh Chem 1997, V128, P571 HCAPLUS
- (3) Amer, A; Monatsh Chem 1998, V129, P1237 HCAPLUS

(44) Babcock, G. Biochemisery 1989, V28, P9557 Heaplus (5) Carpenter, S. Photochemienotobiol 1991, V53, P169 HCAPLUS ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr 154 3

ANSWER 3 OF 61 HCAPLUS COPYRIGHT 2000 ACS L54

1999:23725 HCAPLUS AN

DN 130:95421

ΤI The dissociation and tautomerization equilibria of hypericin. Alkyl-protected hydroxyl derivatives

ΑU

Amer, Atef M.; Falk, Heinz; Tran, Huyen T. N. Institut Chemie, Johannes Kepler Universitaet, Linz, A-4040, Austria

Monatsh. Chem. (1998), 129(12), 1237-1244 CODEN: MOCMB7; ISSN: 0026-9247

Springer-Verlag Wien PR

DT Journal

LA English

3-Benzyl-, 3,4-dibenzyl-, 3,4-dibenzyl-1,6,8,13-tetramethyl-, and AB 1,6,8,13-tetramethylhypericin were synthesized by alkylation and dealkylation procedures starting from hypericin. The pKa value correlation of these derivs. allowed the unequivocal assignment of the protonation and deprotonation pKa values of hypericin. Thus, for hypericin the pKa of .apprxeq.-6 was assigned to the C:O groups, that of .apprxeq.2 to the deprotonation of 1 OH group in the bay-positions 3/4, and that of .apprxeq.9 was found to be characteristic of the bay-peri-diphenolate ion. None of the changes in the spectra characteristic of changes in the tautomeric equil. could be found for these derivs. Thus, it was concluded that the undisturbed peripheral OH groups of hypericin have to be present to allow for tautomeric changes.

219547-31-6P 219547-32-7P 219547-33-8P

219547-34-9P

RL: PEP (Physical, engineering or chemical process); FRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC

(prepn. and deprotonation and tautomerization equil. of alkyl-protected hydroxyl derivs. of hypericin)

RN 219547-31-6 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,6,8,13-pentahydroxy-10,11-dimethyl-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)

219547-32-7 HCAPLUS RN

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,13-tetrahydroxy-3,4dimethyl-10,11-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)

219547-33-8 HCAPLUS RN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,13-tetramethoxy-3,4dimethyl-10,11-bis(phenylmethoxy) - (9CI) (CA INDEX NAME)

RN 219547-34-9 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-dihydroxy-1,6,8,13-CN tetramethoxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RE.CNT 30

RE

- (1) Agostinis, P; Biochem Biophys Res Commun 1996, V220, P613 HCAPLUS
- (2) Ahrer, W; Monatsh Chem 1998, V129, P643 HCAPLUS (3) Altmann, R; Monatsh Chem 1997, V128, P571 HCAPLUS
- (4) Carpenter, S; Photochem Photobiol 1991, V53, P169 HCAPLUS
- (6) Etzlstorfer, C; Monatsh Chem 1993, V124, P923 HCAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr 154 4

- L54 ANSWER 4 OF 61 HCAPLUS COPYRIGHT 2000 ACS
- AN 1998:432997 HCAPLUS
- DN 129:244909
- TI Studies on synthesis and anti-HIV activity of hypericin and ethylhypericin
- AU Zhao, Jin; Zhang, Zhiping; Chen, Hongshan; Chen, Xianghong
- CS Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences, Beijing, 100050, Peop. Rep. China
- Beijing, 100050, Peop. Rep. China SO Yaoxue Xuebao (1998), 33(1), 67-71 CODEN: YHHPAL; ISSN: 0513-4870
- PB Chinese Academy of Medical Sciences, Institute of Materia Media
- DT Journal
- LA Chinese
- AB Condensed polycyclic anthraquinone hypericin and its analogs showed antiretrovirus activities, including human immunodeficiency virus (HIV). Activity of Ethylhypericin synthesized from butanone was compared with hypericin. The ethylhypericin was slightly more effective than hypericin in HIV retrotranscription test.
- IT 213138-46-6P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 - (synthesis and anti-HIV activity of hypericin and ethylhypericin)
- RN 213138-46-6 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-diethyl-1,6,8,10,11,13-hexahydroxy- (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 5

L54 ANSWER 5 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1998:399546 HCAPLUS

DN 129:202778

TI Quantum chemistry calculation study on photosensitization of perylenequinonoid derivatives

AU Zhang, Hong-Yu

CS Dep. Biology, Shandong Normal Univ., Jinan, 250014, Peop. Rep. China

SO Shengwu Huaxue Yu Shengwu Wuli Xuebao (1998), 30(3), 272-276 CODEN: SHWPAU; ISSN: 0582-9879

PB Shanghai Kexue Jishu Chubanshe

DT Journal

LA Chinese

AMI method has been employed to calc. perylenequinonoid photosensitizers (PQDs). Parameters such as heat of formation (HF), HOMO, LUMO levels and spin d. distribution of free radicals are obtained. In combination with exptl. results, several photophys. and photochem. characteristics of PQDs are elucidated, which lay a foundation for investigating photosensitive mechanisms of PQDs further.

IT **41689-58-1**, Isohypericin

RL: PRP (Properties)

(quantum chem. calcn. study on photosensitization of perylenequinonoid derivs.)

RN 41689-58-1 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,6,8,10,13-hexahydroxy-4,11-dimethyl- (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 6

- L54 ANSWER 6 OF 61 HCAPLUS COPYRIGHT 2000 ACS
- AN 1998:348082 HCAPLUS
- DN 129:95350
- TI On the structure of oxyblepharismin and its formation from blepharismin
- AU Spitzner, Dietrich; Hofle, Gerhard; Klein, Iris; Pohlan, Silke; Ammermann, Dieter; Jaenicke, Lothar
- CS Institut fur Chemie, Universitat Hohenheim, Stuttgart, D-70599, Germany
- SO Tetrahedron Lett. (1998), 39(23), 4003-4006 CODEN: TELEAY; ISSN: 0040-4039
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- AB The blepharismins from Blepharisma japonicum give the corresponding oxyblepharismins on irradn. in vitro and in vivo. The chem. structures of these compds. are elucidated and a mechanism is given for this unusual transformation.
- IT 209669-10-3P, Stentorin A 209669-11-4P, Stentorin B 209669-31-8P, Stentorin D 209669-32-9P, Stentorin E RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
 - (structure of oxyblepharismin and formation from blepharismin)
- RN 209669-10-3 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-diethyl-1,3,4,6,8,10,11,13-octahydroxy- (9CI) (CA INDEX NAME)

- RN 209669-11-4 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2-ethyl-1,3,4,6,8,10,11,13-octahydroxy-5-(1-methylethyl)- (9CI) (CA INDEX NAME)

- RN 209669-31-8 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 5-ethyl-1,3,4,6,8,10,11,13-octahydroxy-9-methyl-2-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 209669-32-9 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-9-methyl-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

IT **147395-58-2P**, Stentorin C

RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (structure of oxyblepharismin and formation from blepharismin)

RN 147395-58-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 7

- L54 ANSWER 7 OF 61 HCAPLUS COPYRIGHT 2000 ACS
- 1998:190509 HCAPLUS AN
- DN 128:257278
- ΤI Synthesis and properties of hypericins substituted with acidic and basic residues. Hypericintetrasulfonic acid. A water soluble hypericin derivative
- ΑU Falk, Heinz; Sarhan, Abd-El-Wareth A. O.; Tran, Huyen T. N.; Altmann,
- Inst. Chemie, Johannes Kepler Univ., Linz, A-4040, Austria
 Monatsh. Chem. (1998), 129(3), 309-318 CS
- SO CODEN: MOCMB7; ISSN: 0026-9247
- Springer-Verlag Wien
- DT Journal
- English LA
- AB Sulfonation of hypericin leads to the corresponding di-, tri-, and tetrasulfonates. The latter is water-sol. up to millimolar solns. Homoaggregate formation (J-aggregates) was obsd. only >5.cntdot.10-4mol/l. In aq. soln., the hypericintetrasulfonate exists as its bay-phenolate with most of the sulfonates dissocd. Thus, a water-sol. hypericin deriv., which in contrast to hypericin is not prone to homoassocn., is presented. Hypericintetrasulfonate forms heteroassocs. with serum albumin, DNA, and .gamma.-cyclodextrin. Hypericin derivs. with primary and tertiary amino group appendages at the hypericin Me groups were synthesized. However, upon salt formation or quaternization these derivs. became virtually insol. in all common solvents including water.
- 205384-03-8P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of hypericinsulfonates and amino hypericins)
- 205384-03-8 HCAPLUS
- Acetamide, N,N'-[{7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14dioxophenanthro[1,10,9,8-opqra]perylene-3,4-diyl)bis(methyleneoxy-2,1ethanediyl)]bis- (9CI) (CA INDEX NAME)

- ΙT 205384-04-9P 205384-07-2P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of hypericinsulfonates and amino hypericins)
- RN 205384-04-9 HCAPLUS
- Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis[(2aminoethoxy)methyl]-1,6,8,10,11,13-hexahydroxy- (9CI) (CA INDEX NAME)

OH O OH
$$CH_2-O-CH_2-CH_2-NH_2$$
 $CH_2-O-CH_2-CH_2-NH_2$ OH O OH

RN 205384-07-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[2-(1-piperidinyl)ethoxy]methyl]- (9CI) (CA INDEX NAME)

OH O OH
$$CH_2-O-CH_2-CH_2-N$$

$$CH_2-O-CH_2-CH_2$$

$$OH O OH$$

=> d bib abs hitstr 154 8

L54 ANSWER 8 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1998:190503 HCAPLUS

DN 128:257277

TI Synthesis and properties of ionophore conjugated hypericin derivatives

AU Altmann, Robert; Falk, Heinz; Gruber, Hermann J.

CS Inst. Chemie, Johannes Kepler Univ., Linz, A-4040, Austria

SO Monatsh. Chem. (1998), 129(3), 235-244 CODEN: MOCMB7; ISSN: 0026-9247

PB Springer-Verlag Wien

DT Journal

LA English

AB Two types of derivs. substituted with ionophoric residues at the .omega.,.omega.'-Me groups of hypericin were synthesized. On the one hand, an open-chain triethylene glycol deriv. did not form stable complexes with alkali metal ions. Embedded as its detergent salt in lipid bilayer membranes it did not provide specific H+, Na+, or K+ channels. On the other hand, crown-4 and crown-5 hypericin derivs. were able to complex Na+ and K+ ions, with the crown-5 compd. forming a stable K crown complex. In such systems, the hypericinate ion is intramolecularly compensated by the complexed cation, thereby forming an extremal structure within the series of hypericinates.

IT 171782-06-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and properties of ionophore conjugated hypericin derivs.)

RN 171782-06-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[2-[2-(2-hydroxyethoxy)ethoxy]methyl]- (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 9

L54 ANSWER 9 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1998:74125 HCAPLUS

DN 128:140417

TI Hypericin, hypocrellin, and model compounds: steady-state and time-resolved fluorescence anisotropies

AU Das, K.; Dertz, E.; Paterson, J.; Zhang, W.; Kraus, G. A.; Petrich, J. W.

CS Department of Chemistry, Iowa State University, Ames, IA, 50011-3111, USA

SO J. Phys. Chem. B (1998), 102(8), 1479-1484 CODEN: JPCBFK; ISSN: 1089-5647

PB American Chemical Society

DT Journal

LA English

AB Steady-state and time-resolved fluorescence anisotropies of hypericin (I), hypocrellin (II), and 5 other analogs were measured. The steady-state excitation anisotropies for each of these compds. has a broad min. at .apprx.400 nm with a neg. value. At the blue and red edges of the spectrum the value of the anisotropy is pos. Time-resolved fluorescence-anisotropy measurements were performed for both I and II at excitation wavelengths of 300 and 570 nm. The limiting anisotropies are in excellent agreement with the corresponding steady-state values. These results are discussed in terms of the directions of the transition dipoles connecting the ground state to various excited states. The role of conformational isomers and tautomers in the ground and excited states is also considered.

IT 172226-96-9P 172226-97-0P 172226-98-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (steady-state and time-resolved fluorescence anisotropies of hypericin, hypocrellin and model compds.)

RN 172226-96-9 HCAPLUS

N Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-(9CI) (CA INDEX NAME)

RN 172226-97-0 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5,9,12-tetramethyl- (9CI) (CA INDEX NAME)

RN

172226-98-1 HCAPLUS
Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,13-heptahydroxy-11-methoxy- (9CI) (CA INDEX NAME) CN

=> d bib abs hitstr 154 10

L54 ANSWER 10 OF 61 HCAPLUS COPYRIGHT 2000 ACS 1997:704005 HCAPLUS AN DN 128:11224 Light and phosphorylation-induced conformational change in phytochrome a ΤI and photoinduced electron transfer from stentorin ΑU Wells, Todd Alan CS Univ. of Nebraska, Lincoln, NE, USA (1997) 123 pp. Avail.: UMI, Order No. DA9736958 From: Diss. Abstr. Int., B 1997, 58(6), 3027 DΤ Dissertation LA English AΒ Unavailable ΙT **147395-58-2**, Stentorin RL: BPR (Biological process); BIOL (Biological study); PROC (Process) (light and phosphorylation-induced conformational change in phytochrome a and photoinduced electron transfer from stentorin) RN 147395-58-2 HCAPLUS CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 11

ANSWER 11 OF 61 HCAPLUS COPYRIGHT 2000 ACS L54

ΑN 1997:619494 HCAPLUS

DN 127:307250

ΤI Chiroptical properties and absolute configurations of the hypericin chromophore propeller enantiomers

Altmann, R.; Etzlstorfer, C.; Falk, H. Institut Chemie, Johannes Kepler Universitat, Linz, A-4040, Austria CS SO

Monatsh. Chem. (1997), 128(8/9), 785-793 CODEN: MOCMB7; ISSN: 0026-9247

PВ Springer

DT Journal

I.A English

ΑB The diastereomeric mono- and bis-.omega.-appended (R)-menthyl hypericins were studied by absorption spectroscopy, CD measurements, application of the C2 rule, and semiempirical calcus. The abs. configuration (P) is assigned to the inherently chiral phenanthroperylene quinone chromophore of hypericin, the bay-hypericinate ion, and the 1,6-dioxo tautomer displaying a neg. Cotton effect of their long wavelength absorption band. From these results and according to the pos. chiroptical sign of their long wavelength bands, the abs. configuration (M) could be assigned to the stentorin chromophore in the native pigments.

197156-50-6 197156-51-7 197251-98-2

197251-99-3

RL: PRP (Properties)

(chiroptical properties and abs. configuration of menthyl hypericins)

RN 197156-50-6 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10methyl-11-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)

197156-51-7 HCAPLUS RN

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis([[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)

RN 197251-98-2 HCAPLUS

The state of the s

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10methyl-11-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-,
stereoisomer (9CI) (CA INDEX NAME)

RN 197251-99-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 12

L54 ANSWER 12 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1997:619470 HCAPLUS

DN 127:293065

TI The deprotonation and protonation equilibria of a hypericin derivative in aqueous solution

AU Altmann, R.; Falk, H.

CS Institut Chemie, Johannes Kepler Universitat, Linz, A-4040, Austria

SO Monatsh. Chem. (1997), 128(6/7), 571-583 CODEN: MOCMB7; ISSN: 0026-9247

PB Springer

DT Journal

LA English

AB A hypericin deriv. .omega.,.omega.'-appended at the Me groups with 2 polyethylene glycol moieties (.apprx.23 units long) and capped with acetyl groups was synthesized starting from emodin. This deriv. proved to water-sol. and was investigated by spectrophotometric titrn. and electrophoresis. Deprotonation at the bay-region OH group was obsd. at pKa = 1.6. This was followed by a 2nd deprotonation step of a peri-OH group at pKa = 9.4. This deriv. could be protonated at the CO group at pKa = -5.7. From pKa detns. in H2O/EtOH mixts. the corresponding pKa values of hypericin itself were extrapolated to the aq. phase. This resulted in estd. pKa values of 1.8, 9.2, and -6.0, resp.

IT 197228-68-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (deprotonation and protonation equil. of hypericin deriv. in aq. soln.)

RN 197228-68-5 HCAPLUS

CN Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[(7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxophenanthro[1,10,9,8-opqra]perylene-3,4-diyl)bis(methylene)]bis(.omega.-(acetyloxy)- (9CI) (CA INDEX NAME)

OH O OH

$$CH_2$$
 CH_2
 CH_2

=> d bib abs hitstr 154 13

L54 ANSWER 13 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1997:611643 HCAPLUS

DN 127:307249

TI Concerning the enantiomerization barrier of hypericin

AU Altmann, R.; Etzlstorfer, C.; Falk, H.

CS Institut Chemie, Johannes Kepler Universitat, Linz, A-4040, Austria

Monatsh. Chem. (1997), 128(4), 361-370

CODEN: MOCMB7; ISSN: 0026-9247

PB Springer

DT Journal

LA English

AB The syntheses of .omega.-(R)-menthyl and .omega.,.omega.'-bis-(R)-menthyl derivs. of hypericin were achieved, and the corresponding diastereomers could be sepd. The equil. between the resp. diastereomers are slightly displaced in favor of the chromatog. faster moving ones. Kinetic measurements on these easily equilibrating diastereomers provided an Arrhenius activation energy for the interconversion barrier between the 2 propeller conformers of 83 and 89 kJ/mol. The .omega.-menthyl residues are of minor relevance to the height of this barrier, as is also the case for the bay hydroxyl ionization and quinone tautomerization equil. It was thus concluded that the intrinsic barrier for the propeller conformer enantiomerization of hypericin is in the order of 80 kJ/mol. These results are in accord with those obtained from semiempirical calcns.

T 197156-50-6P 197156-51-7P 197251-98-2P

197251-99-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn., enantiomerization, and kinetics thereof of hypericin menthyl derivs.)

RN 197156-50-6 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10methyl-11-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-,
stereoisomer (9CI) (CA INDEX NAME)

RN 197156-51-7 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis([{5-methyl-2-(1-methylethyl)cyclohexyl]oxy}methyl]-, stereoisomer (9CI) (CA INDEX NAME)

RN 197251-98-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-methyl-11-[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)

RN 197251-99-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]methyl]-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 14

L54 ANSWER 14 OF 61 HCAPLUS COPYRIGHT 2000 ACS 1997:611642 HCAPLUS 127:278101 DN ТT Concerning bay salt and peri chelate formation of hydroxyphenanthroperylene quinones (fringelites) Falk, H.; Mayr, E. Institut Chemie, Johannes Kepler Universitat, Linz, A-4040, Austria CS so Monatsh. Chem. (1997), 128(4), 353-360 CODEN: MOCMB7; ISSN: 0026-9247 Springer DT Journal LA English The bathochromic shifts in the diffuse reflectance UV/Vis spectra of certain fringelite-contg. fossil species and the exceptional chem. stability of the fringelites and their resistance against leaching on a geol. time scale can be understood from the unique complexation behavior of fringelites with transition metal ions. According to an absorption spectroscopic study of the model system fringelite D-alk. earth metal and transition metal ions, fringelites are able to form peri chelate complexes. In addn., fringelites bearing bay hydroxyl groups are able to form polymeric phenolates with transition metal ions as well as with alk. earth metal ions. This behavior leads to a complex network lattice consisting of these polymeric chains crosslinked via chelate coordination of the peri regions to transition metal ions like Fe. 196873-95-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (salt formation and chelation of fringelite) 196873-95-7 HCAPLUS RN

CN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13octahydroxy-, calcium salt (1:1) (9CI) (CA INDEX NAME)

Ca

=> d bib abs hitstr 154 15

- L54 ANSWER 15 OF 61 HCAPLUS COPYRIGHT 2000 ACS
- 1997:590902 HCAPLUS AN
- DN 127:270322
- TΙ Electron Transfer Quenching and Photoinduced EPR of Hypericin and the Ciliate Photoreceptor Stentorin. [Erratum to document cited in CA126:137514]
- ΑU Wells, Todd A.; Losi, Aba; Dai, Renke; Scott, Paul; Anderson, Michael;
- Redepenning, Jody; Park, Su-Moon; Golbeck, John; Song, Pill-Soon Departments of Chemistry and Biochemistry, University of Nebraska, Lincoln, NE, 68588-0304, USA
- so J. Phys. Chem. A (1997), 101(40), 7460 CODEN: JPCAFH; ISSN: 1089-5639
- РΒ American Chemical Society
- DT Journal
- English LA
- Page 366. The names of Michael Anderson and Jody Redepenning have been added to the list of authors.
- TΤ 147395-58-2, Stentorin
 - RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process)
 - $({\tt photoinduced}\ {\tt electron-transfer}\ {\tt quenching}\ {\tt of}\ {\tt hypericin}\ {\tt and}\ {\tt stentorin}$ excited singlet states (Erratum))
- 147395-58-2 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 16

L54 ANSWER 16 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1997:452084 HCAPLUS

DN 127:108798

TI Synthesis of stentorin

AU Cameron, Donald W.; Riches, Andrew G.

CS School of Chemistry, The University of Melbourne, Parkville, VIC. 3052, Australia

SO Aust. J. Chem. (1997), 50(4), 409-424 CODEN: AJCHAS; ISSN: 0004-9425

PB CSIRO

DT Journal

LA English

GΙ

Ι

AB The two isomeric structures I (R1 = H, R2 = CHMe2) and I (R1 = CHMe2, R2 = H) proposed for the photodynamic pigment stentorin were both synthesized for the first time, thereby allowing unambiguous identification of the natural material as I (R1 = H, R2 = CHMe2). Synthesis of these highly condensed arom. systems involved controlled oxidative couplings of the new anthrones II (R3 = CHMe2, R4 = H; R3 = H, R4 = CHMe2), each synthesized by regiocontrolled cycloaddn.

IT 147395-58-2P, Stentorin 192379-26-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (mol. structure of stentorin via regiocontrolled synthesis)

RN 147395-58-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

RN 192379-26-3 HCAPLUS

CN Phenanthro{1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13octahydroxy-2,9-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

IT 162975-31-7P 162975-32-8P 162975-33-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (mol. structure of stentorin via regiocontrolled synthesis)

- RN 162975-31-7 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,10,11,13-hexahydroxy-3,4-dimethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

- RN 162975-32-8 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

- RN 162975-33-9 HCAPLUS
- Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-2,9-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 17

- L54 ANSWER 17 OF 61 HCAPLUS COPYRIGHT 2000 ACS
- AN 1997:266863 HCAPLUS
- DN 126:263812
- TI Concerning the acidity and hydrogen bonding of hydroxyphenanthroperylene quinones like fringelite D, hypericin, and stentorin
- AU Etzlstorfer, C.; Falk, H.; Mayr, E.; Schwarzinger, S.
- CS Institut Chemie, Johannes Kepler Univ., Linz, A-4040, Austria
- SO Monatsh. Chem. (1996), 127(12), 1229-1237 CODEN: MOCMB7; ISSN: 0026-9247
- PB Springer
- DT Journal
- LA English
- AB The strongly enhanced acidity of the bay OH group as compared to the resp. peri OH groups of fringelite D, hypericin, and stentorin could be rationalized on the basis of a vinylogous carboxylate and was nicely corroborated by semiempirical calcns. of the AM1 type. Exptl. data obtained from several independent exptl. methods, like polarized absorption spectroscopy, hole burning, and isotope effects, as well as from semiempirical AM1 and 6-31G level ab initio calcns. conclusively pointed to dissym. H bonding systems in both the peri and bay regions of the corresponding bay phenolate ions.
- IT 147395-58-2, Stentorin
 - RL: PRP (Properties)
 - (acidity and hydrogen bonding of hydroxyphenanthroperylene quinones)
- RN 147395-58-2 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 18

L54 ANSWER 18 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1997:224048 HCAPLUS

DN 126:299578

TI Excited-State Photophysics of Hypericin and Its Hexamethoxy Analog: Intramolecular Proton Transfer as a Nonradiative Process in Hypericin

AU English, D. S.; Zhang, W.; Kraus, G. A.; Petrich, J. W.

CS Department of Chemistry, Iowa State University, Ames, IA, 50011, USA

SO J. Am. Chem. Soc. (1997), 119(13), 2980-2986 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

AB The excited-state photophysics of the light induced antiviral agent, hypericin, are compared with those of its methylated analog, hexamethoxyhypericin. This comparison is instructive in understanding both the ground- and the excited-state properties of hypericin. That the hexamethoxy analog has no labile protons that can be transferred, that it cannot protonate its own carbonyl groups, that it has a reduced fluorescence quantum yield and lifetime with respect to hypericin, and that it exhibits no stimulated emission or, more specifically, rise time in stimulated emission completely support our emerging model of the hypericin photophysics. The results are consistent with the presence of intramol. excited-state proton transfer in hypericin but not in its methylated analog.

IT 168287-28-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (in prepn. of hexamethoxyhypericin)

RN 168287-28-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octamethoxy- (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 19

L54 ANSWER 19 OF 61 HCAPLUS COPYRIGHT 2000 ACS

ΑN 1997:140636 HCAPLUS

ΤI Electron Transfer Quenching and Photoinduced EPR of Hypericin and the Ciliate Photoreceptor Stentorin

Wells, Todd A.; Losi, Aba; Dai, Renke; Scott, Paul; Park, Su-Moon; Golbeck, John; Song, Pill-Soon

Departments of Chemistry and Biochemistry, University of Nebraska, Lincoln, NE, 68588-0304, USA J. Phys. Chem. A (1997), 101(4), 366-372

so CODEN: JPCAFH; ISSN: 1089-5639

PB American Chemical Society

DT Journal

LA English

Time-correlated single photon counting was used to observe dynamic quenching of the hypericin and stentorin excited singlet states. The fluorescence quenching data for hypericin and stentorin were interpreted in terms of electron transfer. The obsd. correlation between free energy change of electron transfer and quenching rate const. suggests that quenching proceeds via electron transfer from hypericin and stentorin to the quenchers. EPR spectra for hypericin, stentorin, and stentorin chromoprotein demonstrated that free radical formation was initiated or enhanced by visible light and that similar radical species were produced in each sample. Furthermore, the EPR signal for stentorin was significantly enhanced by 1,4-benzoquinone, but the overall shape and g-value was unchanged. We suggest that electron transfer in the excited state of these chromophores results in the formation of a cation radical. This electron transfer is a rapid and efficient pathway for deactivation of hypericin and stentorin excited singlet states and should be considered when discussing the photoreactivity of hypericin as a photodynamic agent and of stentorin as the Stentor coeruleus photoreceptor.

147395-58-2, Stentorin

RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process)

(photoinduced electron-transfer quenching of hypericin and stentorin excited singlet states)

RN 147395-58-2 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 20

L54 ANSWER 20 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:684927 HCAPLUS

DN 126:74439

TI Structural aspects and electronic absorption of the hydroxyphenanthroperylene quinones fringelite D, hypericin, and stentorin

AU Etzlstorfer, C.; Falk, H.; Mueller, N.; Tran, T. N. H.

CS Inst. Chem., Johannes Kepler Univ. Linz, Linz, A-4040, Austria

SO Monatsh. Chem. (1996), 127(6/7), 659-668 CODEN: MOCMB7; ISSN: 0026-9247

PB Springer

DT Journal

LA English

AB PPP semiempirical quantum chem. calcns. of absorption spectra were performed for hypericin, fringelite D, stentorin, and their resp. conformers, tautomers, and deprotonated species. The results agree with the exptl. absorption spectra of hypericin, fringelite D, and stentorin, their deprotonated species, and the polarized absorption spectra of an .omega.,.omega.'-long chain appended hypericin deriv. embedded in stretched polyethylene.

IT 122194-30-3 141600-17-1 141600-18-2

147395-58-2, Stentorin

RL: PRP (Properties)

(structural aspects and electronic absorption of hydroxyphenanthroperylene quinones fringelite D, hypericin, and stentorin)

RN 122194-30-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,13-tetrahydroxy-(9CI) (CA INDEX NAME)

RN 141600-17-1 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6-dihydroxy- (9CI) (CA INDEX NAME)

RN 141600-18-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-dihydroxy- (9CI) (CA INDEX NAME)

147395-58-2 HCAPLUS RN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-CN octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 21

- L54 ANSWER 21 OF 61 HCAPLUS COPYRIGHT 2000 ACS
- ΑN 1996:545215 HCAPLUS
- DN 125:275503
- The synthesis and biological evaluation of hypericin analogs. [Erratum to ΤI document cited in CA124:55665]
- ΑU Kraus, G. A.; Zhang, W.; Carpenter, S.; Wannemuehler, Y.
- Dep. Chemistry, Iowa State Univ., Ames, IA, 50011, USA Bioorg. Med. Chem. Lett. (1996), 6(16), 2037 CS
- SO CODEN: BMCLE8; ISSN: 0960-894X
- DT Journal
- LA English
- The second full sentence on p. 2634 is cor. The errors were not reflected in the abstr. or the index entries.
- 168287-28-3P 172226-96-9P 172226-97-0P
- 172226-98-1P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and anti-retroviral activity of hypericin analogs (Erratum))

- 168287-28-3 HCAPLUS RN
- Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-CN octamethoxy- (9CI) (CA INDEX NAME)

RN 172226-96-9 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy- (9CI) (CA INDEX NAME)

RN 172226-97-0 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5,9,12-tetramethyl- (9CI) (CA INDEX NAME)

RN 172226-98-1 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,13-heptahydroxy-11-methoxy- (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 22

L54 ANSWER 22 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:340828 HCAPLUS

DN 125:2971

TI Delivery of nucleic acids to cells for transfection using hypericin-polyamine complexes

IN Lavie, Gad; Prince, Alfred M.

PA New York University, USA; New York Blood Center

SO PCT Int. Appl., 47 pp. CODEN: PIXXD2

DT Patent

LA English

CAN CHIM 1

PAN.	CNT I		•	
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
ΡI	WO 9607731	Al 19960314	WO 1995-US11709	19950905
	W: AU, CA,	JP		
	RW: AT, BE,	CH, DE, DK, ES, F	R, GB, GR, IE, IT, LU,	MC, NL, PT, SE
	US 5824654	A 19981020	US 1994-300725	19940902
	AU 9535894	Al 19960327	AU 1995-35894	19950905
DDAT	UC 1004 200725	10040000		

PRAI US 1994-300725 19940902 WO 1995-US11709 19950905

OS MARPAT 125:2971

AB A method for transfection of cultured mammalian cell is provided. The cell is contacted with a complex of the nucleic acid with a hydrophobic, membrane-binding anion and a polycation. The hydrophobic anion may comprise a polycyclic arom. dione (such a hypericin or its analogs), an anthraquinone, an emodin anthrone deriv., a cercosporine deriv., or a fatty acid; the polycation may comprise polylysine, polyarginine, polyasparagine, or various polyalkyleneamines. Thus, a 36-mer oligodeoxyribonucleotide forms a complex with polylysine and hypericin. The complex is 40-50% assocd. with murine T-lymphoblastoid cells, whereas only .apprx.l% is assocd. when DNA was added to the cells in the absence of hypericin or polylysine. HIV p55 gag expression was inhibited in CEM cell cultures exposed to an antisense phosphorothicate oligonucleotide complexed with hypericin and polylysine, whereas the oligonucleotide alone, hypericin alone, and polylysine alone were relatively ineffective.

IT 177354-95-9 177354-96-0

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(delivery of nucleic acids to cells for transfection using hypericin-polyamine complexes)

RN 177354-95-9 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)

RN 177354-96-0 HCAPLUS

CN Phenanthro [1,10,9,8-opqra] perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 23

L54 ANSWER 23 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:308063 HCAPLUS

DN 125:29419

TI Bioorganic studies of a new photoreceptor structure

AU Orlando, M.; Gross, M. L.

CS MidWest Center Mass Spectrometry, University Nebraska, Lincoln, NE, 68588, USA

SO NATO ASI Ser., Ser. C (1996), 475(Mass Spectrometry in Biomolecular Sciences), 429-434
CODEN: NSCSDW; ISSN: 0258-2023

DT Journal

LA English

AB The aim of this work is to show the importance of using different instrumental techniques in the field of bicorg. research to det. the structure of unknown compds. present at trace levels in bicl. systems. FAB MS and MS/MS were employed to elucidate structural features of a new type of photoreceptor chromophore. Moreover, a new approach for establishing the positions of OH groups in polyhydroxylated mols. has been developed, and the underlying ion chem. understood.

IT 147395-59-3

RL: PRP (Properties)

(bioorg studies of new photorece)

(bioorg. studies of new photoreceptor structure stentorin)

RN 147395-59-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 24

L54 ANSWER 24 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:64173 HCAPLUS

DN 124:175677

TI Syntheses, constitutions and properties of stentorin and isostentorin

AU Falk, H.; Mayr, E.

CS Institute Chemie, Johannes-Kepler Universitat, Linz, A-4040, Austria

SO Monatsh. Chem. (1995), 126(12), 1311-21

CODEN: MOCMB7; ISSN: 0026-9247

DT Journal

LA English

AB Stentorin and isostentorin were synthesized from 2-isopropyl-1,3,6,8-tetrahydroxyanthrone by dimerization and chromatog. sepn. of the resulting regioisomers. The anthrone was prepd. in 4 steps starting from easily available properly substituted benzene derivs.; the overall yield of the stentorins was 11%. The constitutions of stentorin and isostentorin could be unequivocally assigned from the 1H NMR spectra of their potassium salts and were found to be in agreement with those derived recently by means of a rational synthesis. The spectroscopic, dissocn., and acid-base properties in ground and excited states as well as the chiroptical properties of the human serum albumin complexes were investigated and discussed comparing them with resp. data of hypericin, fingelite D, and the natural Stentor pigment.

IT 147395-58-2P, Stentorin 147395-59-3P

173832-00-3P 173832-01-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (syntheses, mol. structures and properties of stentorin and isostentorin)

RN 147395-58-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

RN 147395-59-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, dipotassium salt, stereoisomer (9CI) (CA INDEX NAME)

- RN
- 173832-01-4 HCAPLUS
 Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)-, dipotassium salt, stereoisomer (9CI) CN (CA INDEX NAME)

=> d bib abs hitstr 154 25

L54 ANSWER 25 OF 61 HCAPLUS COPYRIGHT 2000 ACS 1995:959345 HCAPLUS AN 124:55665 DN TI The synthesis and biological evaluation of hypericin analogs Kraus, George A.; Zhang, Weijiang ΑU Dep. Chemistry, Iowa State Univ., Ames, IA, 50011, USA Bioorg. Med. Chem. Lett. (1995), 5(22), 2633-6 CS SO CODEN: BMCLE8; ISSN: 0960-894X DΤ Journal LΑ English GΙ

AB The hypericin analogs I [R1-R3, R5 = Me, R4 = H; R, R3-R5 = H, R2 = Me; R1-R5 = H; R1-R3, R5 = H, R4 = Me; R1, R2, R4, R5 = H, R3 = Me] were prepd. and tested for virucidal activity against equine infectious anemia virus. Although the peri-hydroxyl groups in hypericin are essential for retroviral inhibitory activity, the remaining hydroxyl groups can be alkylated without loss of activity.

IT 168287-28-3P 172226-96-9P 172226-97-0P 172226-98-1P

Ι

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and anti-retroviral activity of hypericin analogs)

RN 168287-28-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13octamethoxy- (9CI) (CA INDEX NAME)

RN 172226-96-9 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-(9CI) (CA INDEX NAME)

172226-97-0 HCAPLUS RN

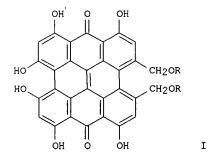
Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5,9,12-tetramethyl- (9CI) (CA INDEX NAME)

RN

172226-98-1 HCAPLUS
Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,13-heptahydroxy-11-methoxy- (9CI) (CA INDEX NAME) CN

=> d bib abs hitstr 154 26

L54 ANSWER 26 OF 61 HCAPLUS COPYRIGHT 2000 ACS 1995:946572 HCAPLUS ΆN DN 124:29512 ΤI On the synthesis of .omega.-appended hypericin derivatives Falk, H.; Vaisburg, A. F.; Amer, A. M. ΑU Inst. Chemie, Johannes Kepler Univ., Linz, A-4040, Austria CS SO Monatsh. Chem. (1995), 126(8/9), 993-1000 CODEN: MOCMB7; ISSN: 0026-9247 DT Journal LA Enalish os CASREACT 124:29512 GI



AB A method for the prepn. of bis-.omega.-appended hypericin derivs. I [R = octyl, hexadecyl, CH2CH2(OCH2CH2)2OH] was developed. The key step, the synthesis of appropriately .omega.-substituted emodin derivs., was achieved by solvolyzing 3-bromomethyl-1,6,8-triacetyloxy-anthracene-9,10-dione (.omega.-bromotriacetylemodin) in the appropriate alc. in the presence of silver perchlorate. I were then prepd. conventionally by dimerizing the .omega.-substituted emodin anthrones. The latter were prepd. by redn. of the .omega.-appended emodins. The soly of I is very similar to that of hypericin.

IT 171782-04-0P 171782-06-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of alkoxy-substituted hypericin)

RN 171782-04-0 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy10,11-bis[(octyloxy)methyl]- (9CI) (CA INDEX NAME)

OH O OH

$$CH_2-O-\{CH_2\}_7-Me$$
 OH
 OH

RN 171782-06-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-bis[[2-[2-(2-hydroxyethoxy]ethoxy]ethoxy]methyl]- (9CI) (CA INDEX NAME)

OH O OH

$$CH_2 - O - CH_2 - OH$$
 $CH_2 - O - CH_2 - CH_2 - CH_2 - CH_2 - CH_2 - CH_2 - OH$
 $CH_2 - O - CH_2 - CH_2 - O - CH_2 - CH_2 - OH$
 $OH O OH$

=> d bib abs hitstr 154 27

L54 ANSWER 27 OF 61 HCAPLUS COPYRIGHT 2000 ACS 1995:882693 HCAPLUS AN DN 123:313580 ΤI Photo-mechanical responses in the unicellular ciliates ΑU Song, Pill Soon Dep. Chem., Univ. Nebraska, Lincoln, NE, 68588-0304, USA Kagaku to Kogyo (Tokyo) (1995), 48(10), 1222-5 CODEN: KAKTAF; ISSN: 0022-7684 CS SO DT Journal; General Review LA Japanese A review with 6 refs. Photoreceptor structure and photochem. function of Stentor coeruleus and Blepharisma japonicum are discussed. ΑB IT 147395-58-2, Stentorin RL: MSC (Miscellaneous) (photomech. responses in unicellular ciliates) 147395-58-2 HCAPLUS Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 28

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L54 ANSWER 28 OF 61 HCAPLUS COPYRIGHT 2000 ACS
     1995:775793 HCAPLUS
AN
     123:169411
DN
ΤI
     Spectroscopic characterization of hypericin and related compounds
     (stentorin)
     Wynn, Jeanne Lenore
ΑU
CS
     Iowa State Univ., Ames, IA, USA
     (1994) 108 pp. Avail.: Univ. Microfilms Int., Order No.: DA9518458
     From: Diss. Abstr. Int., B 1995, 56(2), 789
DT
     Dissertation
LA
     English
AΒ
     Unavailable
     147395-58-2, Stentorin
IT
     RL: PRP (Properties)
         (spectroscopic properties of stentorin in soln.)
RN
     147395-58-2 HCAPLUS
     Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)
CN
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=> d bib abs hitstr 154 29

L54 ANSWER 29 OF 61 HCAPLUS COPYRIGHT 2000 ACS

1995:760462 HCAPLUS AN

DN 123:198504

ΤI A facile synthesis of stentorin, the photoreceptor of Stentor coeruleus

Iio, Hideo; Zenfuku, Kazutaka; Tokoroyama, Takashi ΑU

Fac. Sci., Osaka City Univ., Osaka, 558, Japan Tetrahedron Lett. (1995), 36(33), 5921-4 CS

SO

CODEN: TELEAY; ISSN: 0040-4039

DΤ Journal

LA English

os CASREACT 123:198504

Stentorin, a protozoan photoreceptor, was effectively synthesized via the Ullmann coupling reaction of 5-bromo-2-isopropyl-1,3,6,8tetramethoxyanthraquinone, which was prepd. from 3-isopropyl-2,4-dimethoxy-6-(3,5-dimethoxybenzyl)benzoic acid via intramol. Friedel-Crafts reaction and regioselective bromination.

167961-26-4P TΤ

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (synthesis of stentorin, the photoreceptor of Stentor coeruleus)

167961-26-4 HCAPLUS RN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-CN octamethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

147395-58-2P, Stentorin

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of stentorin, the photoreceptor of Stentor coeruleus)

RN 147395-58-2 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-CN octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 30

L54 ANSWER 30 OF 61 HCAPLUS COPYRIGHT 2000 ACS

AN 1995:758185 HCAPLUS

DN 123:202007

TI Synthesis and properties of fringelite D (1,3,4,6,8,10,11,13-octahydroxy-phenanthro[1,10,9,8,o,p,q,r,a]perylene-7,14-dione)

AU Falk, H.; Mayr, E.

CS Inst. Chem., Johannes Kepler Univ., Linz, A-4040, Austria

SO Monatsh. Chem. (1995), 126(6/7), 699-710 CODEN: MOCMB7; ISSN: 0026-9247

DT Journal

LA English

AB Fringelite D was synthesized from 1,3,6,8-tetramethoxyanthracen-9-ol via two different efficient routes. The first one involved demethylation and subsequent dimerization. The other one started with dimerization to yield octamethylfringelite D and subsequent demethylation. The starting material was prepd. in four steps from com. available educts, the key step being a benzamide ortho-lithiation. The spectroscopic properties of fringelite D were measured and are discussed. The dissoon., deprotonation, and protonation equil. of fringelite D were characterized by their resp. pK values in ground and excited states and compared with those of hypericin. Homo- and heteroassoon. properties of fringelite D were similar to those of hypericin.

IT 168287-28-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (intermediate; prepn. and properties of fringelite D pigment)

RN 168287-28-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octamethoxy- (9CI) (CA INDEX NAME)

=> d bib abs hitstr 154 31

- L54 ANSWER 31 OF 61 HCAPLUS COPYRIGHT 2000 ACS AN 1995:510603 HCAPLUS DN 122:290569 ΤI Synthesis of Stentorin Cameron, Donald W.; Riches, Andrew G. ΑU School Chemistry, University Melbourne, Parville, Victoria, 3052, CS Australia Tetrahedron Lett. (1995), 36(13), 2331-4 CODEN: TELEAY; ISSN: 0040-4039 DT Journal LA English GΙ
- OH O OH CHMe₂
 HO OH OH OH
 R²
 OH O OH I
- AB The two sym. naphthodianthrone structures I (R1 = CHMe2, R2 = H; R1 = H, R2 = CHMe2) proposed for the photodynamic pigment stentorin have both been synthesized, thereby establishing the correctness of structure I (R1 = CHMe2, R2 = H).
- IT 162975-31-7P 162975-32-8P 162975-33-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of stentorin)
 RN 162975-31-7 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,6,8,10,11,13-hexahydroxy-3,4-dimethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

- RN 162975-32-8 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-2,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

162975-33-9 HCAPLUS RN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethoxy-2,9-bis(1-methylethyl)- (9CI) (CA INDEX NAME)

147395-58-2P, Stentorin 147395-59-3P ΙT

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of stentorin)

RN 147395-58-2 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-CN octahydroxy-2,5-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

147395-59-3 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy-2,9-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

=> d bib abs hitstr 17

```
ANSWER 1 OF 1 HEAPTUS COPYRIGHT 2000 ACS 2000:53336 HEAPTUS
     132:88203
DN
ΤI
     Hypericin, hypericin derivatives, and Hypericum extract as specific T-type
     calcium channel blockers, and their use as T-type calcium channel targeted
     therapeutics
     Shan, Jacqueline J.; Wu, Xi-Chen; Pang, Peter K.
IN
     T.; Ling, Lei
     CV Technologies Inc., Can.
     PCT Int. Appl., 33 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
FAN.CNT 1
     PATENT NO.
                            DATE
                      KIND
                                            APPLICATION NO.
     WO 2000002455
                       A1
                            20000120
                                            WO 1999-US14132 19990709
             W: AE, AL,
                     TT, UÀ
             TM, TR,/
                             UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
             MD, RU
                     TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
                     FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, GA, GN, GW, ML, MR, NE, SN, TD, TG

Al 20000201 AU 1999-49581 19990709
             ES, FI,
             CI,
     AU 9949581
PRAI US 1998-92227
                      19980709
     WO 1999-US14132 19990709
os
     MARPAT 132:88203
     Hypericin has been shown to specifically inhibit T-type calcium channel
     activity. Hypericum ext. contg. hypericin also inhibits T-type calcium
     channel activity. Moreover, other chems. in Hypericum ext. showed a
     synergistic effect to hypericin. In view of this, hypericin or
     hypericin-contg. Hypericum ext. can be used as T-channel blockers.
     Hypericum ext., ext. of other species of the Hypericum genus, ext. of
     other plants contg. hypericin, hypericin derivs., hypericin analogs, e.g.
     pseudohypericin, and other \ensuremath{\mathsf{Hypericum}} ext. constituents can be used as
     therapeutics targeted at T-type calcium channels for treatment of diseases
     assocd. with T-channel abnormality. Methods for administering hypericin
     and Hypericum ext. are disclosed.
     9004-10-8, Insulin, biological studies
     RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
        (hyper- and hypoinsulinemia; hypericin, derivs., and Hypericum ext. as
        specific T-type calcium channel blockers and use as T-type calcium
        channel targeted therapeutics)
RN
     9004-10-8 HCAPLUS
CN
     Insulin (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
     52-39-1, Aldosterone
     RL: BPR (Biological process); BIOL (Biological study); PROC (Process).
        (hyperaldosteronemia; hypericin, derivs., and Hypericum ext. as
        specific T-type calcium channel blockers and use as T-type calcium
        channel targeted therapeutics)
RN
     52-39-1 HCAPLUS
CN
     Pregn-4-en-18-al, 11,21-dihydroxy-3,20-dioxo-, (11.beta.)- (9CI) (CA
     INDEX NAME)
```

Absolute stereochemistry.

RN 153-18-4 HCAPLUS
CN 4H-1-Benzopyran-4-one, 3-[[6-O-(6-deoxy-.alpha.-L-mannopyranosyl)-.beta.-Dglucopyranosyl]oxy]-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 482-36-0 HCAPLUS
CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(.beta.-D-galactopyranosyloxy)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 522-12-3 HCAPLUS

CN 4H-1-Benzopyran-4-one, 3-{(6-deoxy-.alpha.-L-mannopyranosyl)oxy}-2-(3,4-dihydroxyphenyl)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 548-04-9 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 548-04-9 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 1617-53-4 HCAPLUS

CN 4H-1-Benzopyran-4-one, 8-[5-(5,7-dihydroxy-4-oxo-4H-1-benzopyran-2-y1)-2-hydroxyphenyl]-5,7-dihydroxy-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN 11079-53-1 HCAPLUS

CN Bicyclo[3.3.1]non-3-ene-2,9-dione, 4-hydroxy-6-methyl-1,3,7-tris(3-methyl-2-butenyl)-5-(2-methyl-1-oxopropyl)-6-(4-methyl-3-pentenyl)-, (1R,5S,6R,7S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 21637-25-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 2-(3,4-dihydroxyphenyl)-3-(.beta.-D-glucofuranosyloxy)-5,7-dihydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 55954-61-5 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-CN (hydroxymethyl)-11-methyl- (9CI) (CA INDEX NAME)

143183-63-5 HCAPLUS
Bicyclo[3.3.1]non-3-ene-2,9-dione, 4-hydroxy-6-methyl-1,3,7-tris(3-methyl-2-butenyl)-5-(2-methyl-1-oxobutyl)-6-(4-methyl-3-pentenyl)-, CN (1R,5S,6R,7S) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 3

- (1) Kikuta; US 5433957 A 1995 (2) Mazur; US 5120412 A 1992
- (3) Noamesi; Planta Medica 1991, V57(Suppl 1), PA55

L21 ANSWER 1 OF 1 HEARING COPYRIGHT 2000 ACS AN 2000:458255 HCAPLUS

Inhibition of human cytochrome P450 enzymes by constituents of St. John's ΤI wort, an herbal preparation used in the treatment of depression

Obach, R. Scott

Drug Metabolism Department, Candidate Synthesis, Enhancement, and Evaluation, Central Research Division, Pfizer, Inc., Groton, CT, USA J. Pharmacol. Exp. Ther. (2000), 294(1), 88-95 CS

CODEN: JPETAB; ISSN: 0022-3565
American Society for Pharmacology and Experimental Therapeutics PB

DТ Journal

English

Com. available St. John's wort (Hypericum perforatum) exts., prepns. that are used in the treatment of **depression**, were examd. for the potential to inhibit human cytochrome P 450 (CYP) enzyme activities, specifically CYPLA2, CYP2C9, CYP2C19, CYP2D6, and CYP3A4. Crude exts. demonstrated inhibition of each of these five enzymes, with CYP2D6, CYP2C9, and CYP3A4 being more sensitive than CYP1A2 and CYP2C19. Exts. were fractionated by HPLC, and each of the fractions was tested for inhibition of these five CYPs to identify individual constituents with inhibitory activity. Several fractions were shown to possess inhibitory activity, including the fractions contg. hyperforin (the putative active antidepressant constituent), I3, II8-biapigenin, and hypericin. Hyperforin and I3,II8-biapigenin were isolated from the ext., and inhibition consts. for the five CYP activities were measured. In addn., three other constituents, hypericin, quercetin, and chlorogenic acid, were tested for inhibitory activity toward the CYP enzymes. The flavonoid compd. I3, II8-biapigenin was shown to be a potent, competitive inhibitor of CYP3A4, CYP2C9, and CYP1A2 activities with Ki values of 0.038, 0.32, and 0.95 .mu.M, resp. Hyperforin was a potent noncompetitive inhibitor of CYP2D6 activity (Ki = 1.5 .mu.M) and competitive inhibitor of CYP2C9 and CYP3A4 activities (Ki = 1.8 and 0.48 .mu.M, resp.). Hypericin also demonstrated potent inhibition of several CYP activities. These in vitro data indicate that St. John's wort prepns. contain constituents that can potently inhibit the activities of major human drug-metabolizing enzymes and suggest that these prepns. should be examd. for potential pharmacokinetic drug interactions in vivo.

548-04-9, Hypericin

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(inhibition of human cytochrome P 450 enzymes by constituents of St. John's wort)

548-04-9 HCAPLUS RN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-CN 10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RE.CNT 23

(1) Bailey, D; Br J Clin Pharmacol 1998, V46, P101 HCAPLUS

(4) Brolis, M; J Chromatogr A 1998, V825, P9 HCAPLUS

(5) Chan, K; J Label Compd Radiopharm 1982, V19, P321 HCAPLUS

MELLER 09/481,572

- (7) deGroot, M; J Med Chem 1999, V42, P4062 HCAPLUS (8) Edwards, D; Clin Pharmacol Ther 1999, V65, P237 HCAPLUS ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L21 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2000 ACS
- 2000:397036 HCAPLUS AN
- DN 133:129833
- ΤI Biochemical activities of extracts from hypericum perforatum L. 5th communication: dopamine-.beta.-hydroxylase-product quantification by HPLC and inhibition by hypericins and flavonoids
- ΑU Denke, Andrea; Schempp, Harald; Weiser, Dieter; Elstner, Erich F.
- Lehrstuhl fur Phytopathologie, Labor fur angewandte Biochemie, Technische Universitate Munchen, Freising-Weihenstephan, 85350, Germany Arzneim.-Forsch. (2000), 50(5), 415-419 CODEN: ARZNAD; ISSN: 0004-4172
- SO
- Editio Cantor Verlag
- DΤ Journal
- LA English
- English

 Exts. from the herb "St. John's wort" (Hypericum perforatum L.) exhibit beneficial effects on patients suffering from mental depressions

 Lack of catecholamine neurotransmitters may be one biochem. mechanism AΒ for this problem under discussion. It has been recently reported that alc. exts. #fon Hypericum perforatum inhibit dopamine-.beta.-hydroxylase (D-.beta.-H) with an I50 or 0.1 .mu.mol/l on the basis of total hypericin content and with an I50 of 21 .mu.mol/l with pure com. hypericin. As test system polarog. den. of oxygen uptake with tyramine as a substrate analog was used. In the present paper the quantification of the enzymic activity and the potential influence of inhibitors are reported using dopamine as substrate and product (noradrenaline) quantification by HPLC. With this test system it could be shown that D-.beta.-H is strongly inhibited by pseudohypericin (I50 = approx. 3 .mu.mol/1) and hypericin (I50 = approx. 5 .mu.mol/1), whereas the I50-values of various flavonoids (quercitrin, isoquercitrin, hyperoside, rutin, quercetin, amentoflavone, kaempferol) are in the range of 50 .mu.mol/l or higher.
- **548-04-9**, Hypericin **55954-61-5**, Pseudohypericin RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (biochem. activities of exts. from hypericum perforatum and dopamine-.beta.-hydroxylase-product quantification by HPLC and inhibition by hypericins and flavonoids)
- 548-04-9 HCAPLUS RN
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

- 55954-61-5 HCAPLUS
- Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-CN (hydroxymethyl)-11-methyl- (9CI) (CA INDEX NAME)

RE.CNT 13

RE

- (1) Abdelnour-Esquivel, A; J Plant Growth Reg 1992, V11, P221 HCAPLUS (2) Blouquit, M; Horm Metab Res 1996, V28, P122 MEDLINE (3) de Paris, P; Biomed Environm Sci 1995, V8, P114 MEDLINE (6) Fritze, J; Rev Neurosci 1993, V4, P63 MEDLINE (10) Porter, J; Natural Toxins 1995, V3, P91 HCAPLUS ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L21 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2000 ACS
- 2000:362574 HCAPLUS ΑN
- DN 132:343347
- ΤI Methods and materials for treating depression and mood disorder with 5-hydroxytryptophan and an ext. of Hypericum perforatum or other extract and vitamins
- IN Cho, Suk H.; Perkes, Lynn
- Melaleuca, Incorporated, USA
- U.S., 4 pp. CODEN: USXXAM so
- DΤ Patent
- English
- FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6068846	A	20000530	US 1999-368789	19990805

PRAI US 1998-95378 19980805

- Methods and materials are provided for the treatment of depression or mood disorder. Specifically, the invention involves the use of 5-hydroxytryptophan and an ext. of e.g. Hypericum perforatum (St. John's Wort) to treat depression or mood disorders when administered orally. In addn., the invention provides less expensive, naturally derived dietary supplements to treat mild to moderate depression or mood disorder.
- 55954-61-5, Pseudohypericin RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (hydroxytryptophan and Hypericum perforatum ext. or other ext. and vitamins for treating depression and mood disorders)
- 55954-61-5 HCAPLUS
- Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-CN (hydroxymethyl)-11-methyl- (9CI) (CA INDEX NAME)

RE.CNT 3

- (1) Bewicke; US 5820867 1998
- (2) Braswell; US 5911992 1999
- (3) Laruelle; US 4472387 1984

- L21 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2000 ACS
- AN 2000:277862 HCAPLUS
- DN 132:298827
- TI Natural composition for the treatment and prevention of depression , containing St. John's wort and folic acid derivatives.
- IN Buchholz, Herwig; Dudda, Angela; Meduski, Jerzy
- PA Merck Patent G.m.b.H., Germany
- SO PCT Int. Appl., 13 pp.
- CODEN: PIXXD2
- DT Patent
- LA English
- FAN.CNT 1

PATENT NO.

KIND DATE

APPLICATION NO. DATE

WO 2000023089

A1 20000427

WO 1999-EP7556 19991008

W: CA, JP, US

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

PRAI US 1998-104710 19981019

- AB A natural compn. comprises St. John's Wort (Hypericum perforatum L.), its exts. of active ingredients and derivs. of dihydro- and tetrahydrofolic acid. This natural formulation is useful for the treatment and prevention of depression with a better effect than the ingredients alone (no clin. data).
- IT **548-04-9**, <u>Hypericin</u>
 - RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (natural compn. for the treatment and prevention of depression , contg. St. John's wort and folic acid derivs.)
- RN 548-04-9 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RE.CNT 2

- RE
- (1) Bewicke, C; US 5820867 A 1998
- (2) Nutramax Lab Inc; WO 9937155 A 1999

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L21
      ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2000 ACS
AN
      1999:819230 HCAPLUS
DN
      132:44995
TI
      Neuroprotective composition for the prevention and/or treatment of nervous
      and behavioral alterations due to anxiety states or depression
ΙN
      Cavazza, Claudio
PA
      Sigma-Tau Healthscience S.p.A., Italy
so
      PCT Int. Appl., 17 pp.
      CODEN: PIXXD2
DΤ
      Patent
LA
      English
FAN.CNT 1
      PATENT-NO.
                           KIND DATE
                                                      APPLICATION NO.
                                                                            DATE
      WO 9966914
PΙ
                            A2
                                   1999122/9
                                                      WO 1999-IT175
                                                                            19990617
          9966914
                            A3
                                   20000406
           W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
                JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
           MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK,
                ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

20000110 AU 1999-43910 19990617

RM425 19880625
      AU 9943910
PRAI IT 1998-RM425
      WO 1999-IT175
                           1/9990617
     A compn. is disclosed for the prevention and/or therapeutic treatment of nervous and behavioral alterations due to anxiety states or
      depression that may take the form of a dietary supplement,
      dietetic support or of an actual medicine which comprises as
      characterizing active ingredients acetyl L-carnitine and hypericin.
      Pharmacol. tests show that, while carnitines alone did not modify
      aggression latency times in mice treated with the, their use in
      combination with either Hypericum ext. of hypericin potentiates the redn.
      in aggression which the latter produce in mice. Pharmaceutical compns.
      contg. the combination were given.
      548-04-9, Hypericin
      RL: BAC (Biological activity or effector, except adverse); THU
      (Therapeutic use); BIOL (Biological study); USES (Uses)
          (neuroprotective compn. for prevention and/or treatment of nervous and \dot{}
         behavioral alterations due to anxiety states or depression)
      548-04-9 HCAPLUS
RN
      \label{eq:phenanthro} Phenanthro [1,10,9,8-opqra] perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
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ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2000 ACS 1999:468883 HCAPLUS AN DN 131:120681 TI A double-blind randomized trial to investigate 3 different concentrations of a standardized fresh plant extract obtained from the shoot tips of Hypericum perforatum AU Lenoir, S.; Degenring, F. H.; Saller, R. St. Gallen, Svitz.
Phytomedicine (1999), 6(3), 141-146
CODEN: PYTOEY; ISSN: 0944-7113 PR Urban & Fischer Verlag Journal DT LA English The efficacy and tolerability was investigated of a new standardized fresh-plant ext. obtained from the shoot tips of St. John's wort (H. perforatum) in the treatment of mild to moderate depression.

Out-patients with mild to moderate depression took during 6 wk 3 times a day 1 tablet of a Hypericum prepn. standardized to either 0.17, AB 0.33, or 1 mg total hyperifin her day. The main outcome measure was the Hamilton Psychiatric Rating Scale for Depression. Addnl. measures were the Hospital Anxiety and Depression Scale and the Clin. Global Impression. At the end of treatment, a redn. in the av. Hamilton Depression score from an initial 16-17 to 8-9 was obsd. in all groups. The response rates were 62, 65, and 68%, resp. Tolerability was excellent, with mild adverse reactions probably causally related to the treatment occurring in only 2% of the patients. The Hypericum prepn. is effective in all 3 doses and is well tolerated. **548-04-9,** Hypericin

(dose-dependant antidepressant activity of a Hypericum prepn.) 548-04-9 HCAPLUS Phenanthro[1,10,9,8-opgra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

RE.CNT 25

- (2) Brockmoller, J; Pharmacopsychiatr 1997, V30, P94 HCAPLUS
- (3) Cott, J; Pharmacopsychiatr 1997, V30, P108 HCAPLUS (9) Hoffmann, J; Z Allg Med 1979, V55, P776 MEDLINE
- (11) Kerb, R; Antimicrob Agents Chemother 1996, V40, P2087 HCAPLUS
- (25) Wheatley, D; Pharmacopsychiatr 1997, V30, P77 HCAPLUS ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2000 ACS

1999:87006 HCAPLUS

DN 130:144040

TI Hypericum for fatigue. A pilot study

Stevinson, Clare; Dixon, M.; Ernst, E.

Dep. Complementary Medicine, School Postgraduate Medicine Health Sciences,

Univ. Exeter, Exeter EX2 4NT, UK Phytomedicine (1998), 5(6), 443-447 CODEN: PYTOEN: ISSN: 0944-7113 Gustav Fischer Verlag

PΒ

DT Journal

LA English

Patients consulting their doctors complaining of fatigue were treated with Hypericum ext. (3 .times. 1 tablet daily) for 6 wk. Compared to baseline values, perceived fatigue was lower after 2 wk of treatment and reduced further after 6 wk. Symptoms of depression and anxiety were also reduced. Nearly half the sample was supposed to be depressed at the start of the trial which was possibly related to fatigue.

548-04-9, Hypericin RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (hypericum for fatigue)

548-04-9 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RE. CNT 9

- (1) Bowling, A; Measuring disease: a review of disease specific quality of life measurement scales 1996
- (4) Linde, K; Br Med J 1996, V313, P253 MEDLINE
- (6) Ridsdale, L; Brit J Gen Pract 1994, V44, P413 MEDLINE
- (7) Shahar, E; J Fam Pract 1990, V31(3), P257 MEDLINE
- (9) Zigmond, A; Acta Psychiat Scand 1983, V67, P361 MEDLINE
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2000 ACS L21

1997:738207 HCAPLUS AN

DN 128:43774

ΤI In vitro receptor binding and enzyme inhibition by Hypericum perforatum extract

AII Cott, J. M.

CS Pharmacologic Treatment Research Program, National Institute of Mental Health (NIMH), National Institutes of Health, Rockville, MD, USA Pharmacopsychiatry (1997), 30(Suppl. 2), 108-112 CODEN: PHRMEZ; ISSN: 0176-3679

PΒ Thieme

DT Journal

LA English

AB

Hypericum perforatum L. Hypericaceae (St. John's wort), has been used since the time of ancient Greece for its many medicinal properties. Modern usage is still quite diverse and includes wound healing, kidney and lung ailments, insomnia and depression. This plant has been known to contain a red pigment, hypericin, and similar compds., which have been assumed to be the primary active constituent(s) in this plant genus. A crude Hypericum ext. was tested in a battery of 39 in vitro receptor assays, and two enzyme assays. A sample of pure hypericin was also tested. Hypericin had affinity only for NMDA receptors while the crude ext. had significant receptor affinity for adenosine (nonspecific), GABAA, GABAB, benzodiazepine, inositol triphosphate, and monoamine oxidase (MAO) A and B. With the exception of GABAA and GABAB, the concns. of Hypericum exact required for these in vitro activities are unlikely to be attained after oral administration in whole animals or humans. These data are consistent with recent pharmacol. evidence suggesting that other constituents of this plant may be of greater importance for the reported psychotherapeutic activity. Alternative pharmacol. mechanisms for Hypericum's antidepressant activity are critically reviewed and the possible importance of GABA receptor binding in the pharmacol. of Hypericum is highlighted. Some of these results have been previously reported (Cott, 1995; Cott, 1996; Cott and Misra, 1997).

548-04-9, Hypericin

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(receptor binding and enzyme inhibition by Hypericum perforatum ext.)

548-04-9 HCAPLUS

 $\label{eq:phenanthro} Phenanthro[1,10,9,8-opqra] perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)$

L21 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:226504 HCAPLUS

DN 124:311186

TI A comparative analysis of the photosensitized inhibition of growth-factor regulated protein kinases by hypericin-derivatives

AU Agostinis, P.; Donella-Deana, A.; Cuveele, J.; Vandenbogaerde, A.; Sarno, S.; Merlevede, W.; de Witte, P.

CS Afdeling Biochemie, Katholieke Universiteit, Louvain, Belg.

SO Biochem. Biophys. Res. Commun. (1996), 220(3), 613-17 CODEN: BBRCA9; ISSN: 0006-291X

DT Journal

LA English

AB The photodynamic inhibitory effect of hypericin and a no. of hypericin-derivs. were investigated in vitro using numerous growth-factor regulated protein kinases including receptor-bound (Insulin-R, EGF-R) and non-receptor (Lyn, c-Fgr, CSK, Syk) protein tyrosine kinases as well as Ser/Thr (PK-C, protein kinase CK-2, CK-1) protein kinases. Modification of the hypericin structure altered significantly the specificity of the protein kinase inhibition. In particular, methylation or attachment of long lipophilic chains to both Me groups of the hypericin mol. strongly enhanced the specificity toward PK-C.

IT 548-04-9, Hypericin 55954-61-5, Pseudohypericin 60483-14-9, Hypericin dicarboxylic acid 120667-79-0 137363-72-5, Gymnochrome B 147593-87-1, 2,5-Dibromohypericin 147593-89-3, 2,5,9,12-Tetrabromohypericin 157301-83-2, Fringelite D 171782-05-1

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (photosensitized inhibition of growth-factor regulated protein kinases

by hypericin derivs.: comparative anal.) ${\rm RN}~~548\text{-}04\text{-}9~~{\rm HCAPLUS}$

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 55954-61-5 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-(hydroxymethyl)-11-methyl- (9CI) (CA INDEX NAME)



60483-14-9 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo- (9CI) (CA INDEX NAME)

RN

120667-79-0 HCAPLUS
Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME) CN

RN 137363-72-5 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,9,12-tribromo-1,3,4,6,8,13-hexahydroxy-10(or 11)-(2-hydroxypentyl)-11(or 10)-(2-hydroxypropyl)-, stereoisomer (9CI) (CA INDEX NAME)

D1-Br

RN 147593-87-1 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dibromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RN 147593-89-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5,9,12-tetrabromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RN 157301-83-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy- (9CI) (CA INDEX NAME)

171782-05-1 HCAPLUS
Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis[(hexadecyloxy)methyl]-1,6,8,10,11,13-hexahydroxy- (9CI) (CA INDEX

OH O OH

$$CH_2-O-(CH_2)_{15}-Me$$
 $CH_2-O-(CH_2)_{15}-Me$
 $CH_2-O-(CH_2)_{15}-Me$

L21 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2000 ACS

AN 1995:620220 HCAPLUS

DN 123:51258

TI Photosensitized inhibition of growth factor-regulated protein kinases by hypericin

AU Agostinis, P.; Vandenbogaerde, A.; Donnella-Deana, A.; Pinna, L. A.; Lee, K.-T.; Goris, J.; Merlevede, W.; Vandenheede, J. R.; De Witte, P.

Fac. Farmaceutische Wetenschappen, Katholieke Univ. Leuven, Belg.

Biochem. Pharmacol. (1995), 49(11), 1615-22 CODEN: BCPCA6; ISSN: 0006-2952

DT Journal

LA English

4

AB

The naphthodianthrone hypericin causes a photosensitized inhibition of protein kinases involved in growth factor signaling pathways. Nanomolar concns. of hypericin inhibit the protein tyrosine kinase activities (PTK) of the epidermal growth factor receptor and the insulin receptor, while being ineffective towards the cytosolic protein tyrosine kinases Lyn, Fgr, TPK-IIB and CSK. Photosensitized inhibition by hypericin is not restricted to receptor-PTKs since the Ser/Thr protein kinases (protein kinase CK-2, protein kinase C and mitogen-activated kinase) are also extremely sensitive to inhibition (IC50 value for protein kinase CK-2=6 nM). A comparison of the hypericin-mediated inhibition of the epidermal growth factor-receptor PTK and protein kinase CK-2 revealed that the inhibition is irreversible, strictly dependent upon irradn. of the enzyme-inhibitor complex with fluorescent light and likely mediated by the formation of radical intermediates (type I mechanism). Although the exact mol. basis for the selectivity of enzyme inhibition by hypericin remains unknown, the results suggest that distinctly related protein kinases could still share common reactive domains for the interaction with hypericin.

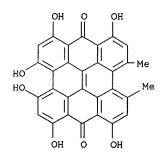
IT 548-04-9, Hypericin

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (photosensitized inhibition of growth factor-regulated protein kinases by hypericin)

RN 548-04-9 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

- L21 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2000 ACS
- 1987:113450 HCAPLUS AN
- DN 106:113450
- Experimental animal studies of the psychotropic activity of a Hypericum extract
- ΑU Okpanyi, S. N.; Weischer, M. L.
- Inst. Pharmakol. Toxikol., Univ. Muenster, Muenster, 4400, Fed. Rep. Ger. Arzneim.-Forsch. (1987), 37(1), 10-13
- CODEN: ARZNAD; ISSN: 0004-4172
- DT Journal
- LA German
- AB Exts. of H. perforatum (Psychotonin M) with known concns. of hypericin [548-04-9] were tested in animal models used for screening psychotropics, and in particular of antidepressant activity. Hypericum Ext. enhanced the exploratory activity of mice in a foreign environment dose-dependently prolonged the narcotic sleeping time, and within a narrow dose range exhibited reserpine antagonism. Similar to most other antidepressants, Hypericum ext. enhanced the activity of mice in the water-wheel test and after a prolonged daily administration decreased aggressiveness in socially isolated male mice. This data in addn. to the already proven clin. efficacy justify the use of standardized Hypericum ext. in the treatment of mild to moderate depression.
- 548-04-9, Hypericin RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (of Hypericum perforatum ext., antidepressant activity of)
- 548-04-9 HCAPLUS
- Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)





153 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2000 ACS AN 1998:487842 HCAPLUS

129:119683 DN

Photoactivated antiviral and antitumor compositions ΤI

Kraus, George A.; Carpenter, Susan L.; Petrich, Jacob W.

Iowa State University Research Foundation, USA PA

U.S., 26 pp. Cont.-in-part of U.S. Ser. No. 995,887, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 3

PATENT NO.

KIND DATE APPLICATION NO. DATE

US 1995-474000 19950607

US 5780287 19980714 PRAI US 1992-995877 19921223

OS MARPAT 129:119683

Disclosed herein are compds., compns., and methods to inactivate a virus and destroy tumor cells. The methods involve the addn. into the cell of a compd. contg. a photosensitizing chem. and an energy-donating chem., optionally linked by a chem. tether. Also introduced into the cell are means to chem. activate the energy-donating chem. which photoactivates the photosensitizing chem. which then destroys the tumor or virus. The photosensitizing chem. is preferably <u>hypericin</u>, <u>porphyrin</u>, or an analog and the energy-donating chem. is preferably luciferin or an analog. Methods for synthesizing the chems. are also disclosed. Further, the energy-donating chem. is activated by an activating chem. The expression of the activating chem. is regulated so as to target the virus-infected or tumor cells. Regulating the activating chem. is accomplished by a no. of methods including construction of an expression plasmid contg. a gene encoding the activating chem. under control of a promoter which is transactivated by replication of the virus or transactivated by elevated levels of proteins expressed in tumor cells.

172226-97-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (photoactivated antiviral and antitumor compns.)

172226-97-0 HCAPLUS RN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13octahydroxy-2,5,9,12-tetramethyl- (9CI) (CA INDEX NAME)

WER 1 OF 10 HEAPLUS COPYRIGHT 2000 ACS

1999:729276 HCAPLUS

132:32711 DN

ΤI Bromohypericins are potent photoactive antiviral agents

ΑU Hudson, Jim B.; Delaey, Els; De Witte, Peter A.

Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, BC, V52 1M9, Can.
Photochem. Photobiol. (1999), 70(5), 820-822
CODEN: PHCBAP; ISSN: 0031-8655 CS

SO

PΒ American Society for Photobiology

DT Journal

LA Enalish

Several hypericin derivs. previously shown to have interesting light-mediated biol. activities, were evaluated for antiviral activities against herpes simplex virus and influenza virus. Three brominated AB hypericins, the dibromo- and tetrabromo-derivs. and the natural compd. gymnochrome B were all very active against both viruses, particularly herpes simplex virus, although light was required in all cases for max. activity. The dibromohypericin was the most potent, under std. assay conditions, gymnochrome B-was approx. as active as hypericin itself and tetrabromohypericin significantly less so. Surprisingly, hexamethylhypericin, which is known to have potent anti-protein kinase (PK) C activity, as well as anticell proliferation properties, showed no antiviral activity at all. The compds. were also evaluated in different serum concns. All the active compds. were inhibited by increasing concns. of serum, but to different degrees, such that their relative antiviral potencies changed to some extent. Thus, in summary, there was no correlation between antiviral and anti-PK or anticellular activities, and consequently it is not possible at present to define those structural features of hypericin-type mols. that are required for their various biol. activities.

120667-79-0 137363-72-5, Gymnochrome B IΤ 147593-87-1 147593-89-3

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (bromohypericins as photoactive antiviral agents)

RN 120667-79-0 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME)

RN 137363-72-5 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,9,12-tribromo-1,3,4,6,8,13-hexahydroxy-10(or 11)-(2-hydroxypentyl)-11(or 10)-(2-hydroxypropyl)-, stereoisomer (9CI) (CA INDEX NAME)

D1-Br

RN147593-87-1 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dibromo-1,3,4,6,8,13hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RN 147593-89-3 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5,9,12-tetrabromo-CN 1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RE.CNT 10

(2) Carpenter, S; Photochem Photobiol 1991, V53, P169 HCAPLUS

(3) Hudson, J; Antiviral Res 1991, V15, P101 HCAPLUS
(4) Hudson, J; Antiviral Res 1993, V20, P173 HCAPLUS
(5) Hudson, J; Photochem Photobiol 1997, V65, P352 HCAPLUS

(6) Hudson, J; Planta Med 1994, V60, P329 HCAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2000 ACS

ΑN 1998:68186 HCAPLUS

DN 128:215036

ΤI Cytotoxicity and antiproliferative effect of hypericin and derivatives after photosensitization

ΑU Vandenbogaerde, Ann L.; Delaey, Els M.; Vantieghem, Annelies M.; Himpens, Bernard E.; Merlevede, Wilfried J.; De Witte, Peter A.

Laboratorium voor Farmaceutische Biologie en Fytofarmacologie, Faculteit Farmaceutische Wetenschappen, Katholieke Universiteit Leuven, Louvain, B-3000, Bela.

Photochem. Photobiol. (1998), 67(1), 119-125 CODEN: PHCBAP; ISSN: 0031-8655

American Society for Photobiology

DT Journal

LA English

The toxicity on three human tumor cell lines (A431, HeLa and MCF7) of five phenanthroperylenequinones (hypericin and derivs.) and two perylenequinones (cercosporin and calphostin C) was investigated after photosensitization (4 J/cm2). Furthermore, the antiproliferative effect on HeLa cells was studied for the phenanthroperylenequinones. Hypericin, 2,5-dibromohypericin, 2,5,9,12-tetrabromohypericin and perylenequinones displayed a potent cytotoxic and antiproliferative effect in the nanomolar range. Hypericin dicarboxylic acid exhibited no photoactivity. In general, the antiproliferative activity correlated well with the photocytotoxicity. However, the nonphotocytotoxic compd. hexamethylhypericin showed potent antiproliferative activity in the nanomolar range, probably exerting its action by protein kinase C inhibition. Without light irradn., no cytotoxic and antiproliferative effect was obsd. for any photocytotoxic phenanthroperylenequinone compd. Furthermore, confocal laser microscopy revealed that the subcellular localization in A431 cells was similar for the photoactive compds.; the photosensitizers were mainly concd. in the perinuclear region, probably corresponding with the Golgi app. and the endoplasmic reticulum. In addn., the accumulation of the photosensitizers in HeLa cells was investigated. All compds. except hypericin dicarboxylic acid were found to conc. to a large extent in the cells. The compd. 2,5,9,12tetrabromohypericin seemed intrinsically more effective than hypericin since the intracellular concn. of the bromoderivative was a magnitude of order lower than that of hypericin although both compds. showed similar photobiol. activity.

60483-14-9, Hypericin dicarboxylic acid 120667-79-0 147593-87-1, 2,5-Dibromohypericin 147593-89-3,

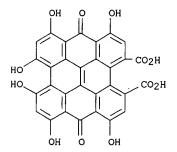
2,5,9,12-Tetrabromohypericin

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(cytotoxicity and antiproliferative effect of hypericin and derivs. after photosensitization)

RN 60483-14-9 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo- (9CI) (CA INDEX NAME)



MELLER 09/481,572

120667-79-0 HCAPLUS RN

1

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME) CN

RN

147593-87-1 HCAPLUS
Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dibromo-1,3,4,6,8,13-CN hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RN 147593-89-3 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5,9,12-tetrabromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME) CN

L35 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2000 ACS

1997:247932 HCAPLUS ΑN

126:303226

Hypericin, Hypocrellin, and Model Compounds: Primary Photoprocesses of Light-Induced Antiviral Agents

English, D. S.; Das, K.; Zenner, J. M.; Zhang, W.; Kraus, G. A.; Larock, AU R. C.; Petrich, J. W.

Department of Chemistry, Iowa State University, Ames, IA, 50011, USA SO

J. Phys. Chem. A (1997), 101(18), 3235-3240 CODEN: JPCAFH; ISSN: 1089-5639

American Chemical Society

DT Journal

I.A English

ΑB The excited-state photophysics of the light-induced antiviral agents hypericin and hypocrellin are compared with those of the hexa- and tetramethoxy analogs of hypericin. The results are consistent with the interpretation of the primary photoprocess in hypericin and hypocrellin as that of excited-state intramol. proton or atom transfer.

189113-18-6P

RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (hypericin, hypocrellin, and model compds.: primary photoprocesses of light-induced antiviral agents)

RN 189113-18-6 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6-tetramethoxy- (9CI) (CA INDEX NAME)

475-64-9 120667-79-0

RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(hypericin, hypocrellin, and model compds.: primary photoprocesses of light-induced antiviral agents)

RN 475-64-9 HCAPLUS

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

MELLER 09/481,572

RN 120667-79-0 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME)

L35 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:664254 HCAPLUS

DN 126:84127

TI Antivirial activity of a derivative of the photosensitive compound hypericin

AU Yip, L.; Hudson, J. B.; Gruszecka-Kowalik, E.; Zalkow, L. H.; Towers, G. H. Neil

CS Dep. Botany, Univ. British Columbia, Vancouver, BC, Can.

SO Phytomedicine (1996), 3(2), 185-190 CODEN: PYTOEY; ISSN: 0944-7113

PB Fischer

DT Journal

LA English

AB Eight synthetic compds. related to the photosensitive antiviral quinonic plant compd. hypericin were screened for light-mediated antiviral activity. 2,5,9,12-Tetra(carboxyethylthiomethyl)hypericin showed activity against membrane-enveloped Sindbis virus and murine cytomegalovirus. The mechanism of action was of the photosensitive singlet oxygen type and the activity could be reduced by the presence of a singlet oxygen quencher mol.

IT 185672-52-0

RL: BAC (Biological activity or effector, except adverse); **THU** (**Therapeutic use**); BIOL (Biological study); USES (Uses) (antiviral activity of photosensitive hypericin deriv.)

RN 185672-52-0 HCAPLUS

Propanoic acid, 3,3',3'','-[(7,14-dihydro-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl-7,14-dioxophenanthro[1,10,9,8-opqra]perylene-2,5,9,12-tetrayl)tetrakis(methylenethio)]tetrakis-(9CI) (CA INDEX NAME)

$$HO_2C-CH_2-CH_2-S-CH_2$$
 OH O OH $CH_2-S-CH_2-CH_2-CO_2H$ $CH_2-S-CH_2-CH_2-CO_2H$ $CH_2-S-CH_2-CH_2-CO_2H$ $CH_2-S-CH_2-CH_2-CO_2H$ $CH_2-S-CH_2-CH_2-CO_2H$



L35 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:333058 HCAPLUS

DN 125:26266

TI Methods and polycyclic aromatic compound containing compositions for treating T-cell-mediated diseases

IN Meruelo, Daniel; Lavie, Gad

PA New York University, USA

SO U.S., 21 pp. Cont.-in-part of U.S. Ser. No. 784, 952, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 55147 <u>14</u>	Α	19960507	US 1993-39790	19930330
110 1000-572005	10000	022		

PRAI US 1990-572085 19900823

US 1991-784952 19911101

A

T cell-mediated diseases in mammals are treated using compns. comprising a polycyclic arom. compd., preferably hypericin or pseudohypericin, and related compds., including isomers, analogs, derivs., salts, or ion pairs of hypericin or pseudohypericin. The above compn. may be administered in combination with an immunosuppressive agent. Pharmaceutical compns. useful for treating a T cell-mediated disease comprise the above polycyclic arom. compd., alone or in combination with an immunosuppressive agent. The compns. and methods are useful in treating diseases which include multiple sclerosis, myasthenia gravis, scleroderma, polymyositis, graft-vs.-host disease, graft rejection, Graves disease, Addison's disease, autoimmune uveoretinitis, autoimmune thyroiditis, pemphiqus vulgaris, psoriasis, systemic lupus erythematosus, and rheumatoid arthritis. Also provided are methods for diminishing the expression of CD4 Mols. on the surface of a T lymphocyte, and for inducing multidrug resistance in a cell, comprising incubating the cell with an effective concn. of a polycyclic arom. compd.

IT 55914-74-4, Hypericin hexaacetate

RL: **THU** (**Therapeutic use**); BIOL (Biological study); USES (Uses) (polycyclic arom. compds. for treating T-cell-mediated diseases)

RN 55914-74-4 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexakis(acetyloxy)-10,11-dimethyl- (9CI) (CA INDEX NAME)

L35 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2000 ACS

AN 1996:226504 HCAPLUS

DN 124:311186

TI A comparative analysis of the photosensitized inhibition of growth-factor regulated protein kinases by hypericin-derivatives

.U Agostinis, P.; Donella-Deana, A.; Cuveele, J.; Vandenbogaerde, A.; Sarno, S.; Merlevede, W.; de Witte, P.

CS Afdeling Biochemie, Katholieke Universiteit, Louvain, Belg.

D Biochem. Biophys. Res. Commun. (1996), 220(3), 613-17 CODEN: BBRCA9; ISSN: 0006-291X

DT Journal

LA English

The photodynamic inhibitory effect of hypericin and a no. of hypericin-derivs. were investigated in vitro using numerous growth-factor regulated protein kinases including receptor-bound (Insulin-R, EGF-R) and non-receptor (Lyn, c-Fgr, CSK, Syk) protein tyrosine kinases as well as Ser/Thr (PK-C, protein kinase CK-2, CK-1) protein kinases. Modification of the hypericin structure altered significantly the specificity of the protein kinase inhibition. In particular, methylation or attachment of long lipophilic chains to both Me groups of the hypericin mol. strongly enhanced the specificity toward PK-C.

IT 60483-14-9, Hypericin dicarboxylic acid 120667-79-0

137363-72-5, Gymnochrome B 147593-87-1,

2,5-Dibromohypericin **147593-89-3**, 2,5,9,12-Tetrabromohypericin **157301-83-2**, Fringelite D **171782-05-1**

RL: BAC (Biological activity or effector, except adverse); THU

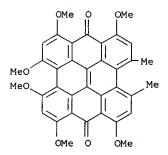
(Therapeutic use); BIOL (Biological study); USES (Uses) (photosensitized inhibition of growth-factor regulated protein kinases by hypericin derivs.: comparative anal.)

RN 60483-14-9 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo- (9CI) (CA INDEX NAME)

RN 120667-79-0 HCAPLUS

CN Phenanthro[1,10,9,8-opgra]perylene-7,14-dione, 1,3,4,6,8,13-hexamethoxy-10,11-dimethyl- (6CI, 9CI) (CA INDEX NAME)



RN 137363-72-5 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,9,12-tribromo-1,3,4,6,8,13-hexahydroxy-10(or 11)-(2-hydroxypentyl)-11(or 10)-(2-hydroxypropyl)-, stereoisomer (9CI) (CA INDEX NAME)

D1-Br

RN 147593-87-1 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dibromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RN 147593-89-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5,9,12-tetrabromo-1,3,4,6,8,13-hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

RN 157301-83-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy- (9CI) (CA INDEX NAME)

171782-05-1 HCAPLUS RN

Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 3,4-bis[(hexadecyloxy)methyl]-1,6,8,10,11,13-hexahydroxy- (9CI) (CA INDEX NAME)

OH O OH

$$CH_2-O-(CH_2)_{15}-Me$$
 $CH_2-O-(CH_2)_{15}-Me$
 OH
 OH
 OH
 OH
 OH
 OH
 OH
 OH
 OH

ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2000 ACS

1996:185233 HCAPLUS AN

124:284089 DN

ΤI Antiviral activities of anthraquinones, bianthrones and hypericin derivatives from lichens

ΑU

Ι

Cohen, P. A.; Hudson, J. B.; Toweres, G. H. N. Dep. Botany, Univ. British Columbia, Vancouver, BC, V6T 1Z4, Can. CS

SO Experientia (1996), 52(2), 180-3 CODEN: EXPEAM; ISSN: 0014-4754

DΤ Journal

LA English

GΙ



II

The antiviral activities of some naturally occurring anthraquinones, bianthrones, and hypericin derivs. were compared by the end-point CPE (viral cytopathic effects) method and plaque assays. Under optimal conditions of exposure to light, hypericin (I), 7,7'-dichloroemodin, and 5,7-dichloroemodin exhibited strong inhibitory activity against HSV-1 (herpes simplex virus type 1) in both assays. Partial inactivation of the virus was shown by emodin (II), 7-chloroemodin and 7-chloro-1-0methylemodin; the bianthrones and other anthraquinones were found to be inactive. Antiviral activity appeared to be pos. correlated with increasing substitution of chlorine in the anthraquinone structure. In the absence of light, only hypericin and 7,7'-dichlorohypericin displayed detectable activity.

164397-06-2

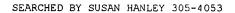
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(antiviral activities of anthraquinones, bianthrones, and hypericin derivs. from lichens)

164397-06-2 HCAPLUS RN

CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 2,5-dichloro-1,3,4,6,8,13hexahydroxy-10,11-dimethyl- (9CI) (CA INDEX NAME)

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L35 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2000 ACS
     1995:826623 HCAPLUS
AN
DN
     123:237784
ΤI
     Inactivation of viruses present in blood components using
     chemically-activated compounds
IN
     Zepp, Charles M.; Heefner, Donald L.
     Hemasure Inc., USA
     PCT Int. Appl., 30 pp.
     CODEN: PIXXD2
DT
     Patent
     English
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                            APPLICATION NO.
                                                             DATE
                                            -----
ΡI
     WO 9518530
                             19950713
                                            WO 1995-US464
                                                             19950109
         W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI,
             GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG,
             MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT,
             UA, US
         RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN,
             TD, TG
                                            CA 1995-2180854 19950109
     CA 2180854
                       AA
                            19950713
                            19950801
     AU 9515658
                       A1
                                            AU 1995-15658
                                                             19950109
                           19961030
     EP 739163
                       A1
                                           EP 1995-907419
                                                            19950109
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                      19940110
PRAI US 1994-179437
     WO 1995-US464
                     19950109
     MARPAT 123:237784
     A method of inactivating viral mols. present within a blood sample and
     compds. for use in inactivation are described. The method involves adding
     to a virus-contg. blood sample an effective quantity of a compd. which
     both has an affinity for viral nucleic acid and which is activatable to an
     excited state in which the compd. covalently binds viral nucleic acid.
     After permitting the compd. to complex with viral nucleic acid, the compd.
     is raised to its excited state by chem. activation. Psoralen, hypericin
     or a deriv. of psoralen or hypericin is used as the activatable,
     viral-inactivating compd., and chem. activation of the compd. is effected
     by the decompn. of a dioxetane proximate to the nucleic acid/compd.
     complex. The activatable, viral-inactivating compd. is then orated into a
     dioxetane mol., and chem. activation of the compd. is effected by decompn.
     of the dioxetane into pair of carbonyl compds.
     168323-98-6
     RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (inactivation of viruses in blood components using chem.-activated
        compds.)
RN
     168323-98-6 HCAPLUS
     Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-10-
     methyl-11-[[[2-[[4-[3-(phosphonooxy)phenyl]spiro[1,2-dioxetane-3,2'-
     tricyclo[3.3.1.13,7]decan]-4-yl]oxy]ethyl]amino]methyl]- (9CI) (CA INDEX
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- L35 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2000 ACS
- AN 1995:615811 HCAPLUS
- DN 123:65629
- TI Hypericin as an inactivator of infectious viruses in blood components
- AU Lavie, G.; Mazur, Y.; Lavie, D.; Prince, A.M.; Pascual, D.; Liebes, L.; Levin, B.; Meruelo, D.
- CS Medical Center, New York University, New York, NY, USA
- SO Transfusion (Bethesda, Md.) (1995), 35(5), 392-400 CODEN: TRANAT; ISSN: 0041-1132
- DT Journal
- LA English

AB

- Hypericin is a potent virucidal agent with activity against a broad range of enveloped viruses and retroviruses. The effective virucidal activity emanates from a combination of photodynamic and lipophilic properties. Hypericin binds cell membranes (and, by inference, virus membranes) and crosslinks virus capsid proteins. This action results in a loss of infectivity and an inability to retrieve the reverse transcriptase enzymic activity from the virion. Since hypericin is devoid of adverse action in most blood components and blood analyses, it is investigated as an additive with potential to inactivate infective viruses in blood components intended for transfusion. Complete inactivation of 106 tissue culture-IDs of human immunodeficiency virus was obtained in whole blood and in dild. packed red cells after illumination with fluorescent light for 1 h. Loss of viral infectivity to cultured CEM cells has been monitored by use of a detection assay for human immunodeficiency virus p55 in ELISA and cytopathic assays. In physiol. media, hypericin interacts with albumin and lipoproteins, retaining the virucidal activity in bound form. The mol. is neg. charged and forms org. and inorg. monobasic salts (ion pairs) in physiol. pH. Various ion pairs differ in virucidal efficacy. The apparent transfusibility of hypericin, taken together with the efficacy of the virucidal activity, the broad range of enveloped viruses affected, and the absence of adverse effects on stored red cells, may render hypericin useful for inactivation of infectious viruses in red cells.
- IT 60935-17-3, Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy- 157301-83-2
 RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 - (hypericin and analogs for virus inactivation in blood preservation)
- RN 60935-17-3 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,13-hexahydroxy-(9CI) (CA INDEX NAME)

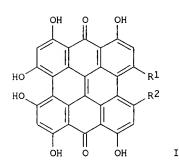
- RN 157301-83-2 HCAPLUS
- CN Phenanthro[1,10,9,8-opqra]perylene-7,14-dione, 1,3,4,6,8,10,11,13-octahydroxy- (9CI) (CA INDEX NAME)

L35 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2000 ACS
AN 1995:354447 HCAPLUS
DN 122:132851
TI Preparation of hypericin dicarboxylate esters as antiviral agents
IN Mazur, Yehuda; Lavie, Gad; Meruelo, Daniel; Lavie, David
PA Yeda Research and Development Co., Ltd., Israel; New York University
SO PCT Int. Appl., 26 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN CONT 1



GΙ

FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE WO 9427952 19941208-WO 1994-US5975 19940527 A1 ΑU, W: CA, JΡ RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE Al 19941220 AU 9472023 AU 1994-72023 19940527 AU 689120 19980326 B2 EP 702669 19960327 EP 1994-921214 19940527 A1 EP 702669 B1 19980729 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE JP 1994-500974 19940527 JP 08510753 T2 19961112 AT 1994-921214 AT 168985 19980815 19940527 F. IL 109807 A1 19981206 IL 1994-109807 19940527 19981216 ES 1994-921214 19940527 ES 2122303 Т3 PRAI US 1993-68379 19930527 WO 1994-US5975 19940527 MARPAT 122:132851



AB Title compds. I (R1, R2 = alkyl, R302C wherein R3 = alkyl, the chain of which is optionally interrupted by one or more O, S, and at least 1 of R1 and R2 is R302C). Emodic acid anthrone in MeOH contg. H2SO4 was refluxed for 4 h to give emodic acid anthrone Me ester which in pyridine and piperidine to which was added pyridine N-oxide and FeSO4.7H2O were refluxed for 3 h at 100.degree. to give after workup I (R1 = R2 = MeO2C). Virucidal activity was demonstrated. Pharmaceutical compns. are claimed (no data).

1T 160919-80-2P 160919-81-3P 160919-82-4P

160919-83-5P 160919-84-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); **THU (Therapeutic use)**; BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of hypericin dicarboxylate esters as antiviral agents)

RN 160919-80-2 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, dimethyl ester (9CI) (CA INDEX NAME)

RN 160919-81-3 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, dipropyl ester (9CI) (CA INDEX NAME)

RN 160919-82-4 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, dibutyl ester (9CI) (CA INDEX NAME)

RN 160919-83-5 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, bis(2-methoxyethyl) ester (9CI) (CA INDEX NAME)

RN 160919-84-6 HCAPLUS

CN Phenanthro[1,10,9,8-opqra]perylene-3,4-dicarboxylic acid, 7,14-dihydro-1,6,8,10,11,13-hexahydroxy-7,14-dioxo-, bis[2-(2-methoxyethoxy)ethyl] ester (9CI) (CA INDEX NAME)

MELLER 09/481,572

=> d bib abs hitstr 135 11

10 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE The answer numbers requested are not in the answer set. ENTER ANSWER NUMBER OR RANGE (1):end